

Ivar Tustervatn Berre

Estimation of the Energy Recovery and Emission Potential of Typically Incinerated Norwegian Waste Classes

Master's thesis in Energy & Environmental Engineering

Supervisor: Corinna Schulze-Netzer

Co-supervisor: Candy Anquetil-Deck

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Faculty of Information Technology and Electrical Engineering
Department of Energy and Process Engineering



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Problem Description

This master thesis aims to estimate the elemental composition and related emissions of Norwegian waste classes that are typically sent to incineration. The first aim is to statistically analyze and combine experimental data points to gain insights into the typical chemical composition and heating value of the waste fractions in Norway. This analysis aims to quantify how inhomogeneous the data and results for the different waste classes are. Based on the data analysis, the second aim is to formulate a surrogate composition for each waste class for further investigation and numerical representations in detailed chemistry simulations. New surrogate species are to be included where these are necessary. This is done using a stochastic reactor model.

Abstract

A great challenge for waste-to-energy power plants is their uncertain and variable feedstock, which can lead to the power plants not being run as efficiently as possible, leading to reduced energy output and control of emissions. A way to describe the feedstock is to use surrogates. This is a method where the hundreds or thousands of different species of a feedstock are modelled using a few surrogate species, enabling the feedstock's modelling. The surrogates also provide an estimation of the HHV and the fraction of biomass, oil-based waste and inorganics.

This thesis formulated surrogates for waste classes typically incinerated, using a linear least-square solution between available surrogate species and experimental values. Most of the species used were from two existing models in the literature, but three new species were created to improve the representation of some waste classes containing fossil-originated wastes, rubber and PET. These were made by creating reactions based on experimental data from the literature and then testing these reactions under pyrolysis conditions in a stochastic reactor model.

The surrogates for the waste classes were formulated by first dividing the waste into components and then finding the surrogate formulation for each component. There were found surrogates for 41 components, which were used to create the surrogate formulation for 30 waste classes. It was found that most of the surrogates modelled the elemental composition accurately compared to experimental values. A statistical overview of the experimental and model data for the waste classes was also created. This overview is relevant for stakeholders in waste management and for other research, such as life-cycle analysis.

Sammendrag

En stor utfordring for søppelforbrenningsanlegg er variasjon og usikkerhet angående brenselet. Dette kan føre til at forbrenningsanleggene ikke kjører optimalt, noe som kan redusere energi-produksjonen og kontroll på utslippene. Brenselet kan beskrives ved å bruke surrogater. Dette er en metode hvor de hundre eller tusenvis av ulike stoffene i et brensel blir forklart ved hjelp av noen få surrogatstoffer, som gjør det enklere å modellere brenselet. Surrogatene gir et anslag av øvre brennverdi samt fraksjonene av biomasse, oljebasert avfall og uorganiske stoffer.

Denne masteroppgaven fant surrogater for avfallsklasser sendt til forbrenning ved å bruke en minste kvadraters løsning mellom surrogatstoffene og eksperimentelle verdier. De fleste surrogatstoffene var fra to eksisterende modeller i litteraturen, men tre nye stoffer ble lagd for å forbedre formuleringen av avfallsklasser som inneholdt avfall fra fossile kilder, gummi og PET. De nye stoffene ble lagd ved å lage reaksjoner basert på eksperimentelle data fra litteraturen, for så å teste disse reaksjonene under pyrolyseforhold i en stokastisk reaktor modell.

Surrogatene til avfallsklassene ble funnet ved å først dele avfallet i komponenter, for så å finne surrogatene til hver komponent. Det ble funnet surrogater til 41 komponenter, som deretter ble brukt til å lage surrogater for 30 avfallsklasser. Resultatene viste at surrogatene representerte komposisjonen til avfallsklassene nøyaktig sammenlignet med eksperimentelle verdier. En statistisk oversikt av de eksperimentelle og modellerte verdiene for avfallsklassene ble også lagd. Oversikten er relevant for interessenter i avfallsbransjen og for annen forskning, f.eks. livsløpsanalyse.

Preface

The process of writing this master's thesis has been interesting, enlightening, and sometimes a bit difficult. Still, I am left with much knowledge within the field of waste incineration and the composition of waste.

I would like to thank my supervisors, Corinna Schulze-Netzer and Candy Anquetil-Deck, for their great guidance throughout the semester. My fellow students also deserve thanks for being great company throughout the master period. Finally, I would like to thank my partner Juni for her great support and for holding up with (un)interesting speeches about subjects like the protein content of grass and chlorine content of food waste.

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1 Introduction

In 2021, 11.6 million tons of waste was generated in Norway [1], and the government's goal is to recycle as much of it as possible [2]. However, much of the waste generated today is not recycled due to some waste being too challenging or expensive to recycle. This means that much of the waste generated is not recycled into new materials [1]. Waste-to-energy power plants are therefore an important part of Norway's waste management since they can provide energy that would otherwise not be utilized while reducing the volume of waste sent to landfills. In addition, incinerating the waste reduces the amount of the potent greenhouse gas methane that would have been released if the waste had been directly deposited in a landfill [3].

Several types of combustion systems exist for waste-to-energy power plants, such as moving grate furnaces, fluidized bed combustion and rotary kiln, where the moving grate furnace is the most common today [4]. Waste incineration usually occurs between 1000°C and 1300°C. This is because with a temperature above 1000°C, chemicals like dioxins, which are extremely toxic [5], are destroyed, but a temperature above 1300°C might affect the composition and formation of ash [4]. The residues from the incineration process are slag and ash, which are removed from the bottom of the furnace, as well as flue gases. Waste-to-energy power plants require significant control and cleaning of the flue gases. This is because waste incineration can produce harmful substances such as NO_x, which cause photochemical smog, sulfur oxides (SO_x), which are harmful to people and can cause acid rain, and hydrochloric acid (HCl) and dioxins, which can cause corrosion to the power plants' equipment as well as acid rain [6]. Primary measures, such as reburning and air staging, and secondary measures (cleaning the flue gas after combustion), are used to clean waste incineration emissions. Primary measures are generally less expensive and easier to implement than secondary measures.

To implement primary measures efficiently, precise modelling of the feedstock is necessary. However, a great challenge for waste-to-energy power plants is the uncertainty and variety regarding the feedstock. In Norway, the waste generated is divided into numerous waste classes based on their composition [7], and many of these are typically incinerated [8]. More information about the waste can make it less challenging to predict the energy available in the feedstock, which can improve the prediction of the power plants' energy output. Furthermore, more information about the waste might also be beneficial for implementing secondary measures since it makes it possible to have a more precise prediction of the emissions formed, and one can thus set up the secondary measures accordingly.

A solution for modelling the feedstock more precisely is using a surrogate model to describe the waste classes. Surrogates can describe the numerous species found in a feedstock using only a few surrogate species. Surrogates are widely used within the field of liquid fuel combustion, where complex fuels often are described using a few surrogate species. An example is the octane number, which is determined using a surrogate, namely the ratio between n-heptane and iso-octane [9]. Describing a waste class using surrogates makes it easier to model the incineration process using numerical methods since the input of species in the model is reduced to a couple of surrogate species. The numerical methods can provide information on how to run the power plant more efficiently. In addition, the surrogates can provide information such as the heating value and amount of fossil carbon sources in a feedstock. The use of surrogates has been used for describing biomass, such as woody biomass [10] and algae biomass [11], and it has also been done for sewage sludge [12] and municipal solid waste [6]. However, it is not widely used for describing waste, and, to the author's best knowledge, there are no articles in the open literature regarding surrogates for waste beside the two mentioned above.

The objective of this master thesis is to find a surrogate formulation for waste classes typically sent to incineration in Norway based on the experimental data found in the author's project work [8]. This was done by first dividing the waste classes into different components, which was done in the project work [8]. Then, the surrogates for each waste component are found using available surrogate species from the literature [6, 12]. In addition, new surrogate species are created and used where necessary. The surrogates are formulated in section 3.5. The reactions of the new surrogate species are created based on experiments from the open literature. It is validated by simulating the pyrolysis of the surrogate species using a stochastic reactor model in LOGERsearch and then

comparing the thermogravimetric's from the simulation with experimental data. This is done in section 3.6. Lastly, the higher heating value (HHV), nitrogen, sulphur and chlorine levels from the surrogates were compared to the experimental values for each waste class, and these results can be found in section 4.

A flow chart showing the process used for finding the surrogates for each waste class can be seen in Figure 1.

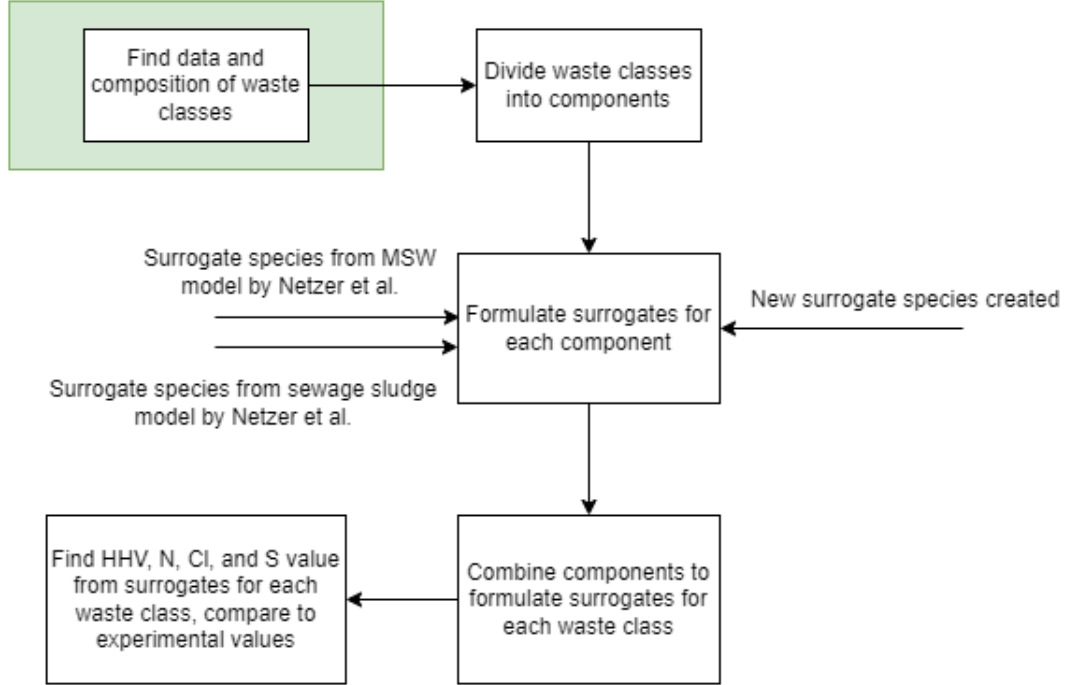


Figure 1: Flow chart of the process of finding the surrogates for each waste class, the green box was done in the author's project work [8]

Source: MSW model by Netzer et al. [6], Sewage sludge model by Netzer et al. [12]

2 Theory

2.1 Waste Classes

In Norway, the waste generated is categorized into numerous waste classes [7]. This is done to safely and efficiently transport, recycle, incinerate and dispose different types of waste. Each waste class is given a four-digit number, with the first or first two digits indicating the category. In total, there are 16 different categories which can be found in Table 1 [7].

Table 1: Digits indicating what a waste class contains

Source: Norsk Standard[7]

Digit(s)	Category	Digit(s)	Category
11	Biological waste and sludge	12	Paper and cardboard
13	Glass	14	Metals
15	Waste electrical and electronic equipment	16	Soil and inorganic materials
17	Plastics	18	Rubber
19	Textiles, leather, furniture and furnishing	22	Chemicals
23	Batteries	24	Means of transport
3	Radioactive waste	6	Medical waste
7	Hazardous waste	99	Mixed waste

This master thesis only focuses on the waste classes that are typically incinerated, as described in the author's project work [8]. A description of each waste class explained in the project work can be found in appendix A. The heterogeneity of the waste classes can vary significantly, from waste classes containing only one component to those containing numerous components. Examples of fairly homogeneous waste classes are 1141 (untreated wood) and 1619 (asphalt), while waste class 9911 (mixed household waste) and 1506 (toys, recreational and sports equipment) are examples of heterogeneous waste classes [7].

The waste classes can be divided into what components they consist of, making it easier to find the elemental composition and formulate the surrogates. The components used in this thesis can be found in section 3.2.

2.1.1 Chemical Waste Properties

The ultimate analysis is the determination of the sample's composition [13], and in this master thesis, the elements of interest are carbon, hydrogen, oxygen, nitrogen, sulphur and chlorine. In addition, the ash and moisture content is provided from proximate analysis [14]. The results from an ultimate analysis can be given as received (all elements, in addition to ash and moisture), dry (all elements, in addition to ash) and dry ash-free (only elements) [14].

The heating value can be given as either the lower or higher heating value. The higher heating value gives the heating value assuming all products are returned to the original pre-combustion temperature [15], which means that the energy of condensation is included. For the lower heating value, it is not assumed that all products are returned to the pre-combustion temperature, and the energy of condensation is therefore not included [15].

2.2 Surrogate Model

A surrogate model is a way of describing the hundreds or thousands of different species in a feedstock by only using a couple of representative species, while the main chemical and physical properties of the feedstock are still represented. Using surrogates enables modelling the incineration of the feedstock, which can give more information about the energy output and emissions [16]. The surrogates can, for example, be used as the input in a stochastic reactor model, which is described in more detail in section 2.3.

The surrogate species used in this thesis, except those created in section 3.6, are the same as those used in models regarding municipal solid waste (MSW) and sewage sludge by Netzer et al. [6, 12]. The surrogate species from these models are the following:

Cellulose ($C_6H_{10}O_5$): Cellulose is a structural component in the primary cell wall of plants and is most often the main component of woody biomass [17]. The reaction and reaction rate for cellulose is based on a model from Ranzi et al. [10].

Hemicellulose ($C_5H_8O_4$): Hemicellulose is a structural component in the primary cell wall of plants. There are many different forms of hemicellulose, such as xylenes and mannans [18]. Here, the chemical formulae ($C_5H_8O_4$) is used [6]. The reaction and reaction rate for hemicellulose is based on a model from Ranzi et al. [10].

Lignin (Oxygen-rich, hydrogen-rich and carbon-rich): Lignin can be found in the cell walls of plants, where it is bounded to cellulose [19]. Lignin is a complex polymer whose chemical structure can vary [20]. Therefore, lignin is divided into three different surrogate species, oxygen-rich lignin, LIG_O ($C_{20}H_{22}O_{10}$), hydrogen-rich lignin, LIG_H ($C_{22}H_{28}O_9$), and carbon-rich lignin, LIG_C ($C_{15}H_{14}O_4$) [6]. The reaction and reaction rate for the lignin species is based on a model from Ranzi et al. [10].

Protein: Proteins are large molecules found in all living things and are made up of smaller parts called amino acids [21]. The size and shape of proteins vary significantly, Netzer et al. used the surrogate species PROT described as $C_{400}H_{900}O_{150}N_{86}$ in their model for MSW [6]. However, in the model for sewage sludge, three protein species were used to improve the description of proteins [12]. There, protein rich in hydrogen, $PROT_H$ ($C_{400}H_{900}O_{150}N_{86}$) (same as PROT), protein rich in carbon, $PROT_C$ ($C_{500}H_{450}O_{65}N_{80}$), and protein rich in oxygen, $PROT_O$ ($C_{250}H_{500}O_{200}N_{72}$) was used. The reaction and reaction rate for all these surrogate species is based on a model from Debiagi et al. [11]

Sugar ($C_6H_8O_6$): Sugars are a class of carbohydrates, and there are several different types of sugar. In the model from Netzer et al. [12], sugar is described as $C_6H_8O_6$ based on a model from Debiagi et al. [11], the reaction and reaction rate are from the same model.

Lipid ($C_{18}H_{32}O_2$): Lipids are a large group which includes substances like fats and waxes [22]. In the sewage sludge model from Netzer et al. [12], lipid is described as $C_{18}H_{32}O_2$ based on a model from Debiagi et al. [11], the reaction and reaction rate are from the same model.

Inorganic nitrogen (NH_3): Inorganic species of nitrogen are described by using ammonia in the MSW model by Netzer et al. [6]. Ammonia models the product gases of the involved species, neglecting the inorganic species itself. The reaction and reaction rate for the inorganic nitrogen is from a model by Debiagi et al. [11].

Inorganic carbon (CO_2): Inorganic species of carbon are described by using carbon dioxide in the MSW model by Netzer et al. [6]. Carbon dioxide models the product gases of the involved species, neglecting the inorganic species itself. The reaction and reaction rate for the inorganic carbon is from a model by Debiagi et al. [11].

Sulphur species (H_2S SO_2 COS): A sulphur species is added to account for the sulphur that might be present in the waste. The sulphur species' reaction rate is from the MSW model by Netzer et al. [6]. As for inorganic carbon and nitrogen, the sulphur species models the product gases of the involved species, neglecting the species itself. The reaction and reaction rate for the sulphur is from the same model by Netzer et al. [6]. For simplicity is this surrogate species called

sulphur in the rest of the thesis.

Polyethene, PE ($[\text{C}_2\text{H}_4]_n$): Polyethene is the most used type of plastic in the world [23]. It is a polymerization of ethylene and is used for making products like home appliances, packaging, bottles and pipes [23]. The reaction for the polyethene species is from the MSW model by Netzer et al. [6], while the reaction rate is from a model by Wu et al. [24].

Polypropylene, PP ($[\text{C}_3\text{H}_6]_n$): Polypropylene is a polymer of propylene and is used for making products such as household appliances, packaging and textiles [25]. The reaction for the polypropylene species is from the MSW model by Netzer et al. [6], while the reaction rate is from a model by Wu et al. [24].

Polystyrene, PS ($[\text{C}_8\text{H}_8]_n$): Polystyrene is a polymer of the aromatic hydrocarbon styrene and is used for making products such as packaging, toys, and styrofoam [26]. The reaction for the polystyrene species is from the MSW model by Netzer et al. [6], while the reaction rate is from a model by Wu et al. [24].

Polyamide, PA ($[\text{C}_6\text{H}_{11}\text{NO}]_n$): Polyamide is a polymer of amides, and it occurs naturally in wool and silk, but can also be synthetically produced [27]. The polyamide species used by Netzer et al. [6] is a synthetic polyamide with the chemical formulae $\text{C}_6\text{H}_{11}\text{NO}$. Polyamide is used for making products such as textiles, carpets, and sportswear [27]. The reaction for the polyamide species is from the MSW model by Netzer et al. [6], while the reaction rate is from a model by Herrera et al. [28].

Polyvinyl chloride, PVC ($[\text{C}_2\text{H}_3\text{Cl}]_n$): PVC is a polymer of vinyl chloride and is a rigid plastic but can be made soft by using plasticizers such as phthalates [29]. It is used for making products such as bottles, pipes, cables, and packaging [29]. The reactions for the polyvinyl chloride species are from the MSW model by Netzer et al. [6], while the reaction rate are from a model by Wu et al. [24].

Water (moisture) and ash: Are included when describing the waste classes. However, these are not included when creating the surrogates but can be added afterwards to give the surrogates on an as-received or dry basis.

In addition to these surrogates, three new surrogate species were formulated in this thesis, and information about these can be found in section 3.6.

For each surrogate species, single or multi-step reaction systems describe their devolatilization. The reactions from the solid species are devolatilization reactions or heterogeneous reactions between solid and gas. The gas phase reactions are homogeneous and cover phenomena such as tar cracking and further oxidation [10]. Kinetic parameters from the Arrhenius equation, seen in Equation 1, determine each reaction [30]. These were found using data from the open literature for the new species created in section 3.6.

$$k = Ae^{-\frac{E_a}{RT}} \quad (1)$$

where,

k: rate constant

A: frequency factor [1/s]

E_a : activation energy [kJ/mol]

R: Universal gas constant

T: Temperature [K]

Following the model by Netzer et al. [6], the surrogates in this master thesis are formulated using a linear-least square fit toward ultimate analysis measurements. This leads to surrogates which resembles the amount of carbon, hydrogen, oxygen, nitrogen, sulphur and chlorine for each data point. Furthermore, since the heating value and emission are closely related to the composition of the elements, the surrogates will most likely predict both of these precisely if they are based on the ultimate analysis.

When formulating the surrogates, some of the species are combined. For example, in the model from Netzer et al. [6], cellulose and hemicellulose are added to form Bio-1. Bio-1 consists of 60% cellulose and 40% hemicellulose and is created since cellulose and hemicellulose have almost the same elemental composition. Therefore, a linear least-square fit could assign a disproportional amount of cellulose or hemicellulose to the surrogate formulation. Because of this, they are combined to form Bio-1, such that the proportion between cellulose and hemicellulose follows results from the literature [31]. The merging of the surrogate species used in the model by Netzer et al. [6] is shown in Equation 2 to 6

$$\text{Bio-1} = 0.6 \cdot \text{CELL} + 0.4 \cdot \text{HCE} \quad (2)$$

$$\text{Bio-2} = 0.8 \cdot \text{LIGH} + 0.2 \cdot \text{LIGC} \quad (3)$$

$$\text{Bio-3} = 0.8 \cdot \text{LIGO} + 0.2 \cdot \text{LIGC} \quad (4)$$

$$\text{Bio-n} = 0.5 \cdot (\text{NH}_3)_i + 0.5 \cdot \text{PROT} \quad (5)$$

$$\text{Plastic-1} = 0.8 \cdot \text{PE} + 0.2 \cdot \text{PP} \quad (6)$$

The surrogate species are able to describe the different elemental ratios of the data points. As an example, Figure 2, 3 and 4 shows how the species from section 2.2 cover the area of a H/C, O/C, N/C, S/C and Cl/C plot. Bio-1, Bio-2, Bio-3, Bio-n and Plastic-1 used in the model from Netzer et al. [6] are used in the figures.

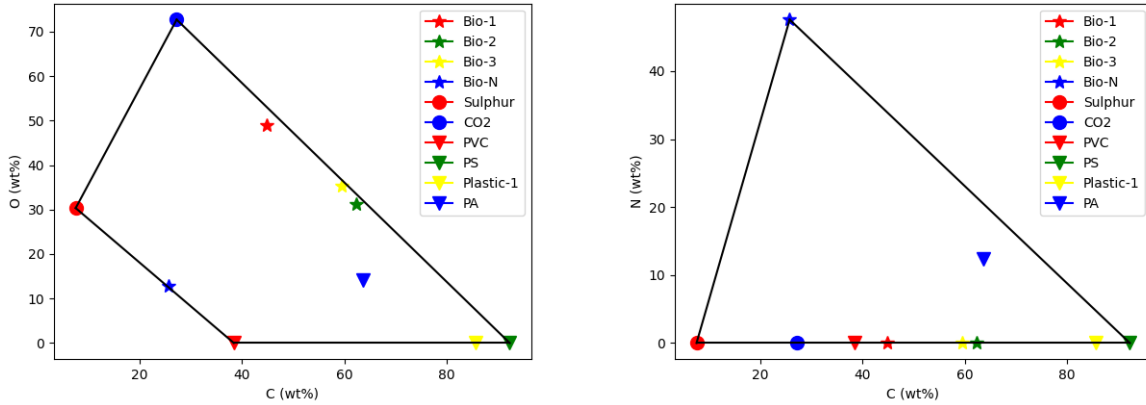


Figure 2: Area that the surrogate species covers on a O/C and N/C plot

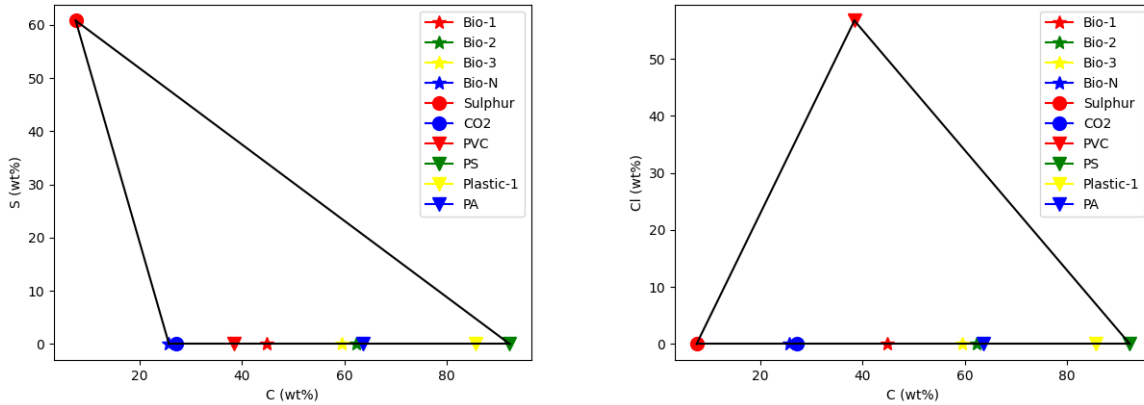


Figure 3: Area that the surrogate species covers on a S/C and Cl/C plot

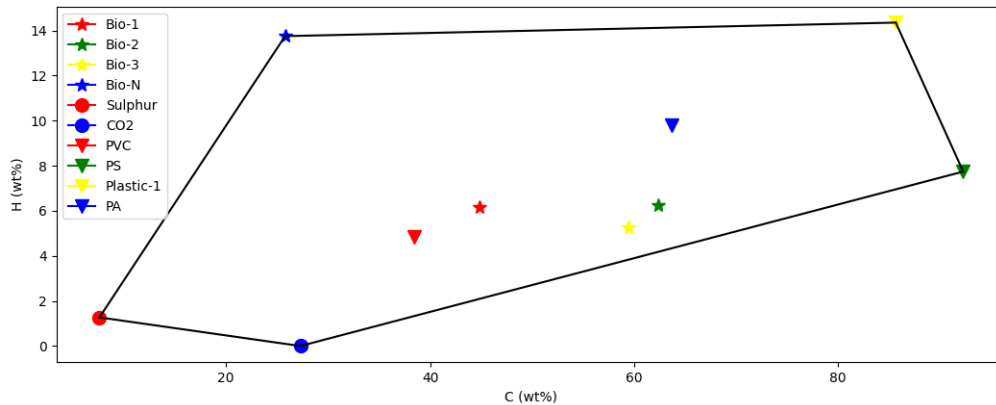


Figure 4: Area that the surrogate species covers on a H/C plot

2.3 Stochastic Reactor Model

Modelling the devolatilization, pyrolysis and incineration processes of different feedstocks is complicated because the processes include chemical reactions, phase changes, and heat and mass transfer, all while being turbulent. The most detailed method of describing these processes is computational fluid dynamics (CFD) simulations, which require significant computing power [32]. Therefore, it might be time-consuming to run these simulations, if they are feasible to run at all.

A stochastic reactor model described by Weber et al. [33] can be used to model the processes more efficiently. In a stochastic reactor model, the turbulent mixing is modelled by a mixing model and the thermal conversion process is driven by chemical reactions [33]. A mixing model mimics the turbulence and mass exchanges of the fluid elements. The model is zero-dimensional and therefore has no spatial information. The stochastic reactor model has explicit non-dimensional particles, and each stochastic particle consists of a combination of solid mass, pore gas (gas trapped inside the solid) and bulk gas (not trapped inside the solid). Figure 5 shows how heat and mass are transported within the model. The chemical reactions drive the mass release from the solid, and this depends on the initial conditions. The initial conditions can be set to be air or pure N_2 combustion.

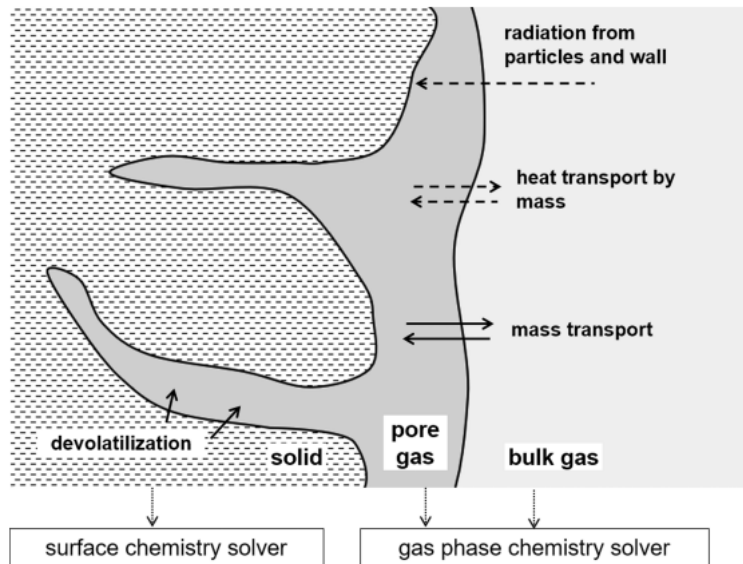


Figure 5: Model schematic

Source: Netzer et al. [32]

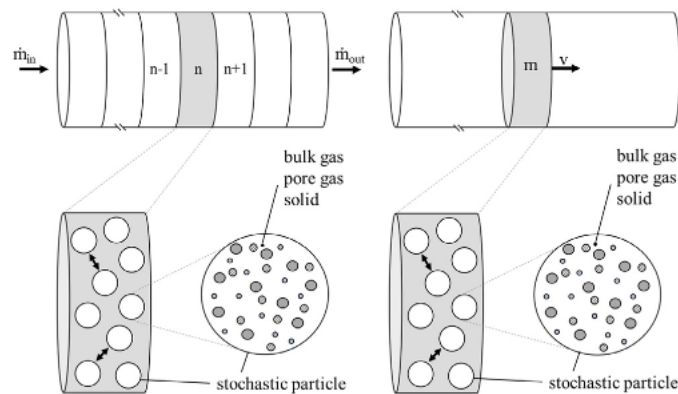


Figure 6: SRM with series of cells (left-hand side) and disc cell (right-hand side)

Source: Weber et al. [33]

Figure 6 shows two different methods of the stochastic reactor model from Weber et al. [33]. The method on the left-hand side of the picture shows how it can be set up as several cells, each with stochastic particles inside them. In addition, the inflow and outflow of solid and gaseous species are considered between the cells. Therefore, finite mixing is accounted for in the radial and axial directions.

In the method on the right-hand side of Figure 6, a disk cell is transported along the length of the reactor. The disk cell is a partially stirred reactor with an initial mass-to-gas ratio. The disk cell consists of several stochastic particles. Since there is no inflow and outflow, like the solution on the left-hand side, this approach only accounts for finite mixing in the radial direction. This thesis uses the setup with the moving disk cell when testing the new surrogates species in section 3.6.

A more detailed and mathematical explanation of the stochastic reactor model is presented by Weber et al. [33].

Netzer et al. [32] used the stochastic reactor model from Weber to model the fuel bed in grate-fired furnaces by combining several different stochastic reactors into a network representing the fuel bed. Therefore, the model presented by Netzer et al. [32] can be used to model the whole incineration

process and predict the emissions from waste incineration.

In this master thesis, new surrogate species and their reactions are created in section 3.6, which can be added to this model for future work. The pyrolysis of the new surrogate species will be modelled using the SRM and pure nitrogen atmospheres.

Figure 7 shows how the emissions can be modelled using surrogates and a numerical model. Each waste class is described using surrogate species described in section 2.2. The figure only shows the waste class being divided into two surrogate species for simplicity. In reality, numerous surrogate species can be used in order to describe the waste classes. Also, many waste classes will be divided into their components described in section 3.2. This would add another step to the figure, dividing each waste class into components. Then the components would be described by their surrogates.

The surrogates can be used in a numerical model, such as the stochastic reactor model, to predict the emissions released by incinerating a waste class [34]. Changing variables such as temperature and amount of air in a numerical model is often possible. Therefore, it is possible to find the conditions that make the incineration process run optimal regarding both the energy output and emissions. It is also possible to include several waste classes, thus modelling the more complex feedstock used at waste-to-energy power plants. This can be done by adding another waste class in the first step of Figure 7.

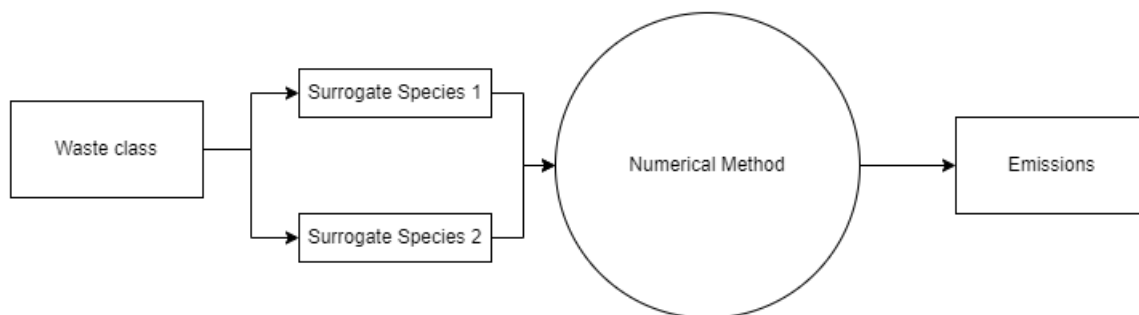


Figure 7: Flow chart of how surrogates can be used to model emissions

2.4 Box Plot

When describing the results in this thesis, the HHV, nitrogen, sulphur and chlorine levels will be presented using box plots. Therefore, this section includes a short explanation of the box plot. A box plot showcases the 5-number summary of a data set, namely the minimum and maximum range values, the upper and lower quartiles, and the median [35].

In order to explain the box plot, the following example is used: Table 2 shows the height of a hypothetical class (the height were assigned randomly by the author). The data from Table 2 is then used to create the box plot seen in Figure 8. The box plot then visualizes the following values [35]:

Table 2: Height of a hypothetical class

Height [cm]
160, 170, 175, 176, 180, 180, 180, 181, 182, 183, 183, 185, 187, 190, 191, 195, 205

Upper and lower quartile: The lower quartile is the value under which 25% of the data is found when sorting them in increasing order. The upper quartile is the value under which 75% of the data is found when sorting them in increasing order [36]. The upper and lower quartiles can be found as the upper and lower edge of the box in the box plot seen in Figure 8.

Minimum and Maximum: The minimum is defined as the first datum greater than (Q1-

$\text{whis} \cdot \text{IQR}$) [37]. $Q1$ is the value of the lower quartile, while IQR is the interquartile range, the distance between the upper and lower quartile. whis stands for whisker, which is a user-defined number. In this thesis, a default value of 1.5 is used [37]. The minimum can be seen as a line extending beneath the box in the box plot, as shown in Figure 8.

The maximum is found using the same principles, only that the maximum is the first datum less than $Q3 + \text{whis} \cdot \text{IQR}$. The maximum can be seen as a line extending over the box in the box plot, as shown in Figure 8.

Outliers: The outliers are data that fall outside the maximum and minimum just described. These are white dots over and under the maximum and minimum in Figure 8.

Mean and median: The median is the value under which 50% of the data is found when sorting in increasing order, and can be seen as the solid yellow line in Figure 8. In addition to the median, the mean (average) is included in the box plots and can be shown as the dotted line in Figure 8.

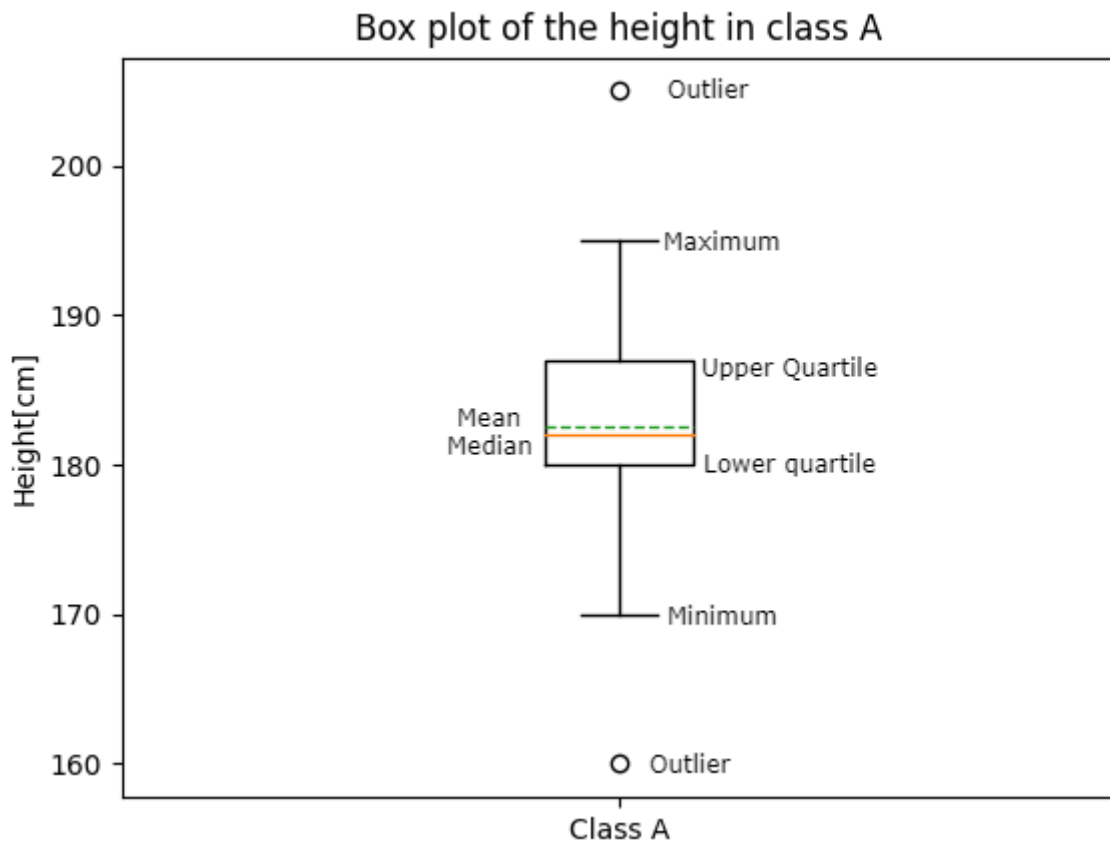


Figure 8: Example of box plot

3 Method Development

3.1 Process for Creating Surrogate Formulations

To formulate the surrogates for each waste class, they were first divided into components, explained in section 3.2. Then the data from the project work was inserted into the model. The process for transferring the data and handling data points missing information is explained in section 3.3. Finally, the surrogate formulation had to be made for each component, which was done using the following steps.

1. Create a surrogate formulation based on the surrogate species from the models by Netzer et al. [6, 12]
2. Adjust limits and ratios of the surrogate species and exclude irrelevant species, if relevant
3. Identify and add new needed surrogate species, if relevant.

Section 3.5.1 demonstrates how the surrogates were created for woody biomass. This level of detail is not included for the other categories, but it has been done following the same procedure. A summary of how the surrogates were formulated is presented for each category. The process of creating new surrogate species is explained in section 3.6, and three new surrogate species were created in this thesis. In the end, the components were put back together to create the results presented in section 4.

The process for formulating the surrogates is visualised as a flow chart in Figure 1. The Python scripts used for creating the surrogates are available in a database [38].

3.2 Components of Waste Classes

In this thesis, the surrogates for Norwegian waste classes typically incinerated, as explained in the author's project work [8], were to be found. However, as described in section 2.1, many Norwegian waste classes are highly heterogeneous and consist of several different components. The description for each waste class was taken from the author's project work [8] and can be found in appendix A. For example, waste class 1506 (toys, recreational and sports equipment) consists of several components such as plastics, paper and wood. Finding the surrogates of waste classes containing several components with considerably different compositions would be difficult. The exception was heterogeneous waste classes with experimental data for the waste class as a whole instead of for each component, such as mixed household waste [38]. This was not the case for many of the waste classes, and for these, the surrogates were formulated for each component. These components were combined to create the results for each waste class in section 4.

Splitting the waste classes into components can simplify finding the surrogates of waste classes with varying components. This is because one can change the amount of each component to receive the value of the waste class. For example, in the author's project work [8], it was assumed that waste class 1751 (composites) consisted of 43% glass fibre, 28.5% carbon fibre and 28.5% mix of composites. By finding the surrogates for each of the three components, one can easily change the ratio of each component to receive the combined surrogates for the waste class.

The different components used can be seen in Table 3 and were based on the description from the author's project work [8]. One can see that many of the waste classes only consist of one component, while some exist of several.

Table 3: Components used to describe the different waste classes.

Waste Class	Components used
1111 - Kitchen and food waste from large- and small-scale households	Organic domestic waste
1126 - Sludge, organic	Sewage sludge, Paper sludge, Food sludge
1131 - Park and garden waste	Park wood, Grass, Leaves and Needles
1141 - Untreated wood	Untreated wood
1142 - Treated wood	Treated wood
1143 - Wood chips, shavings, bark	Wood Chips, Bark, Sawdust
1149 - Mixed treated wood	Mixed treated wood
1504 - Cables	Cables
1506 - Toys, recreational and sports equipment	PVC, PP, PE, PS, PET, Paper, Untreated wood
1621 - Roofing felt/tar paper	Asphalt, Glass fibre plastics
1751 - Composites	Glass fibre plastics, Carbon fibre plastic
1811 - Passenger car tyres	Passenger car tyres
1812 - Tractor and lorry tyres	Truck tyres
1814 - Other tyres	MC/Bike tyres
1899 - Mixed rubber	Mixed rubber waste
1911 - Textiles and leather	Textiles, Synthetic textiles, Leather
1912 - Furniture and furnishing	Furniture wood
2431 - Leisure craft	Glass fibre plastics
6004 - Non-infectious waste	Hospital waste
7021 - Oil and grease	Oil
7022 - Materials contaminated with oil	Textiles, Paper, Oil
7024 - Oil filters	Oil, Paper, Mixed rubber waste
7098 - CCA-treated wood	CCA-treated wood
7142 - Oil-based drilling mud	Diesel
7143 - Cuttings with oil-based drilling mud	Oil cuttings
7152 - Organic waste without halogens	Tar, Distillation residues, Activated carbon
7154 - Creosote-treated wood	Creosote treated wood
7156 - Waste containing phthalates	PVC
9911 - Mixed household waste	Municipal solid waste
9913 - Sorted combustible waste	Refuse-Derived fuel

To formulate the surrogates more efficiently, the components were divided into categories. The categorisation was based on what the different components are made of. For example, all woody biomass were in the same category. The components were divided into categories based on the author's understanding of them. The categories and their components can be seen in Table 4.

Table 4: Categorization of components

Category	Components
Woody biomass	Park wood, leaves and needles, grass, untreated wood, treated wood, wood chips, sawdust, bark, mixed treated wood, paper, textiles, furniture wood, CCA-treated wood, creosote-treated wood
Sludge and other biomass	Organic domestic waste, sewage sludge, paper sludge, leather
Plastics	Cables, PVC, PP, PE, PS, PET, glass fibre plastic, carbon fibre plastic, synthetic textiles
Rubber	Passenger tyres, truck tyres, MC/Bike tyres, rubber waste
Oil-based wastes	Asphalt, oil, diesel, oil-based cuttings, tar, activated carbon, distillation residue
Mixed waste	Municipal solid waste (MSW), refuse-derived fuel (RDF), hospital waste

Not all waste classes contained enough data to create a surrogate formulation. As described in section 3.3, at least two out of three values for carbon, hydrogen and oxygen had to be recorded to obtain the surrogates. The waste class 7051 (paints, glues and varnishes) did not have any data points to create a surrogate formulation [39]. The waste classes for which it was not formulated surrogates are listed in Table 5. This is due to the fact that these mostly consist of inorganic materials, so creating accurate surrogates with the available surrogate species would be difficult [39].

Table 5: Waste classes not included

Waste Class	Waste Class
1603 - Slightly polluted soil, inorganic materials etc.	1604 - Polluted soil, inorganic materials etc.
1606 - Polluted dredging soil	1614 - Polluted concrete and tiles
1671 - Cinders, dust, bottom ash and fly ash	1672 - Blasting sand
7051 - Paints, glues and varnishes	

3.3 Handling of Missing Data

To model each data point using the surrogate species described in section 2.2 and the method described in section 3.5, one had to know the ultimate analysis on a dry ash-free basis for each data point. These values were collected from the database [39], created for the author's project work [8]. However, not all data points contained all the values needed for formulating surrogates. Therefore the following assumptions and calculations were used for the following scenarios:

Moisture content not specified: If the moisture content was not specified, it was set to zero. This did not affect the formulation of the surrogates since it only used values on a dry ash-free basis. Nevertheless, the as-received values calculated from the surrogates could become inaccurate since moisture is set to zero, even though the moisture content might be much higher in reality.

Ash contents not given: If the ash content was only given on an as-received or dry basis, the other value was calculated using Equation 7 [14].

$$Ash_{dry}(wt\%) = \frac{Ash_{ar}(wt\%)}{1 - \frac{Moisture(wt\%)}{100}} \quad (7)$$

If the ash content was not given, but the elements in the ultimate analysis were given in the dry state, Equation 8 was used to find the ash content in the dry state. One could then also find the ash content in the as-received state using Equation 7

$$Ash_{dry}(wt\%) = 100 - C_{dry}(wt\%) - H_{dry}(wt\%) - O_{dry}(wt\%) - N_{dry}(wt\%) - S_{dry}(wt\%) - Cl_{dry}(wt\%) \quad (8)$$

If the ash content was not specified and could not be calculated as described above, it was set to zero. As for the moisture level, this did not affect the formulation of the surrogates but could give inaccurate values if one were to calculate values in the dry state based on the surrogates.

Elemental composition not specified as dry-ash free: If the elemental composition was specified on a dry or as-received basis, it was possible to convert it using Equation 9 and 13 [14].

$$C_{dry}(wt\%) = \frac{C_{ar}(wt\%)}{1 - \frac{Moisture(wt\%)}{100}} \quad (9)$$

$$C_{daf}(wt\%) = \frac{C_{dry}(wt\%)}{1 - \frac{Ash_{dry}(wt\%)}{100}} \quad (10)$$

Here Carbon has been used as an example, but the equation is also valid for the other elements.

Missing Nitrogen, Sulphur or Chlorine: These elements most often constituted a minuscule part of each data point. Therefore it was assumed that it was possible to formulate the surrogates even when one or more of these elements were missing. Because of this, the values of nitrogen, sulphur and chlorine were set to zero if no value was given for either of the three states (daf, dry, ar).

Missing Carbon, Hydrogen or Oxygen value: Carbon, hydrogen and oxygen were the main elements of most data points. Therefore, having these three values to formulate the surrogates was necessary. If one of these values was missing (for daf, dry and ar) while the other two were present, one could find the missing element using Equation 11, where carbon has been used as an example.

$$C_{daf}(wt\%) = 100 - H_{daf}(wt\%) - O_{daf}(wt\%) - N_{daf}(wt\%) - S_{daf}(wt\%) - Cl_{daf}(wt\%) \quad (11)$$

In Equation 11, sulphur, nitrogen and chlorine were set to zero if not given. Therefore all data points containing at least two out of three values of carbon, hydrogen and oxygen for any state (daf, dry or ar) could be used to create a surrogate model.

Missing experimental HHV: To compare the heating value obtained using the surrogates with the experimental heating value, one had to know each data point's heating value in the dry ash-free state. As described in section 2.1.1, two different heating values could be used. For simplicity, only one was used when comparing the heating values. In this thesis, the higher heating value (HHV) was used. This was because the HHV represents the maximum amount of available thermal energy from the combustion of the feedstock [15]. Therefore, it is the greatest amount of energy that could be obtained with complete combustion and exploitation of the latent heat of condensation of the combustion products. However, not all data sets contained the experimental HHV in the dry ash-free state, but several equations exist to find this value. Equation 12 and 13 shows how to find the HHV for each state based on the HHV obtained for different states [14].

$$HHV_{ar} = HHV_{dry} \cdot \left(1 - \frac{Moisture(wt\%)}{100}\right) \quad (12)$$

$$HHV_{dry} = HHV_{daf} \cdot \left(1 - \frac{Ash_{dry}(wt\%)}{100}\right) \quad (13)$$

Equation 14 and 15, show how to go between the HHV and LHV [14].

$$HHV_{dry} = LHV_{dry} + (2.443 \cdot 8.936 \cdot \frac{H_{dry}(wt\%)}{100}) \quad (14)$$

$$HHV_{ar} = LHV_{ar} + (2.443 \cdot 8.936 \cdot \frac{H_{dry}(wt\%)}{100} \cdot \left(1 - \frac{Moisture(wt\%)}{100}\right) + \frac{Moisture(wt\%)}{100}) \quad (15)$$

For some data points the experimental heating values was not available. In order to compare these data to the heating value from the surrogates, approximations of the heating values were needed. In this thesis, the heating value correlation of Channiwala and Parikh was used because it offers a good approximation of the heating value for data with widely different ultimate compositions [40]. The correlation can be seen in Equation 16, where all values of the elements and ash are given in weight per cent on a dry basis.

$$HHV_{dry} = (0.3491 * C) + (1.1783 * H) - (0.1034 * O) - (0.0151 * N) + (0.1005 * S) - (0.0211 * ash) \quad (16)$$

The correlation works well within the limits of 0 - 92.25% for carbon, 0.43 - 25.15% for hydrogen, 0 - 50% for oxygen, 0 - 5.6% for nitrogen, 0 - 94.08% for sulphur and 0 - 71.4% for ash [40]. This means the calculated HHV might be inaccurate for data points where some elemental values are outside the limits.

3.4 Surrogate Formulation

The surrogates for each data point were created optimising a linear combination of the surrogate species towards the experimental ultimate analysis on a dry-ash-free basis [6]. Three methods were tested to formulate the surrogates. These are described in section 3.4.1. They all used a linear least square fit against the experimental ultimate analysis, just with variations in the optimisation target. Limits on each surrogate species to control the amount of each species in the model were applied.

The HHV of each data point was calculated using the composition of surrogate species and the higher heating value of each species. The higher heating value of the surrogate species was calculated using the heating value correlation from Channiwala and Parikh [40], seen in Equation 16. Since the inorganic carbon, nitrogen and sulphur species were given as the gas product they would create, their heating value will not necessarily be correct. This might affect the results later if some of the surrogates contained significant amounts of these. Also, as explained previously, the correlation from Channiwala and Parikh [40] has limits regarding the amount of each element. All the protein species, the inorganic nitrogen, and the PA species had nitrogen levels above these limits, and this might have affected the results for surrogates containing high amounts of these species. The sugar and inorganic carbon species had oxygen levels above the limit, which might also affect the results for surrogates containing high amounts of these species.

The ash and moisture content were added after the optimisation, and then the surrogates of each data point was given with the ash and moisture content included. However, in this thesis, all results are presented on a dry-ash-free basis since many of the input data did not include values for the ash and moisture. Nevertheless, the ash and moisture content is given for each data point in the database [38].

3.4.1 Methods for Formulating Surrogates

In this master thesis, three different methods for formulating the surrogates were considered. All methods used a linear least-square fit between the surrogate species and the experimental values of the data points. The difference between the models was the experimental values used. Table 6 shows the values used for each method.

The first method was based on a model by Netzer et al. [6].

The second method was comparable to the first one with the exclusion of oxygen. The oxygen was added afterwards based on the oxygen content of the surrogates used. This method might be beneficial since one less variable was used, and eventual inaccuracies regarding the oxygen content from experiments were removed. Also, the hydrogen and carbon level is the most important values affecting the dry-ash-free HHV [40]. Since the most important values in this thesis were the HHV, N, S and Cl levels, discarding oxygen might give adequate results.

Table 6: Values used for each method

Method	Elements used
Method 1	Carbon, hydrogen, oxygen, nitrogen, sulphur, chlorine
Method 2	Carbon, hydrogen, nitrogen, sulphur, chlorine
Method 3	Carbon, hydrogen, oxygen, nitrogen, sulphur, chlorine, higher heating value

For the third method, the HHV value was added. This method might give more precise results since the HHV was included as an extra variable in the linear least-square solution.

In order to find the best method, they were all applied to the component untreated wood. Untreated wood was chosen because this was the component containing the greatest amount of data points. The surrogate species and merging of species from the model by Netzer et al. [6] were used, and these are described in section 2.2.

Table 7 shows the average value for each element compared to the average from the experimental values. One can see that Method-1 provided the average values closest to the experimental values, except for nitrogen, where Method-2 was closest, and the HHV, where Method-3 was closest.

Figure 9a shows that the surrogates for each data point matched the experimental HHV values for Method-1 and Method-3, except for some outliers. It can be seen that Method-2 did not match the experimental values for many of the data points. Figure 9b shows that the surrogates for Method-1 and Method-3 matched the experimental carbon and oxygen level. It can also be seen that Method-2 did not match the experimental values. Figure 10a shows that the surrogates for Method-1 matched the experimental hydrogen values, except for data points with high hydrogen content. The surrogates for Method-2 and Method-3 did not match the experimental values. Figure 10b shows that the surrogates for Method-1 and Method-2 matched the experimental values, while Method-3 did not. Table 8 shows an overview of how each method matched the experimental values.

Based on the results shown in Table 7 and Figure 9a to 10b, it was decided to continue with Method-1 for the rest of the thesis. This was due to Method-1 having accurate average values compared to the experiments, while it also predicted each data point well, except for data points with high hydrogen levels. Method-2 produced inaccurate results compared to Method-1 and 3 and was therefore not considered. Method-3 proved to be about as accurate as Method-1, with its HHV values being more accurate. However, Method-3 used the experimental HHV in assigning the surrogates, which can provide inaccurate results for some data points. The inaccuracies were because the experimental heating values for some of the data points in the project work did not match the heating value correlation from Channiwala and Parikh [40]. This might indicate that either the elemental values from the ultimate analysis were inaccurate or that the heating values measured were inaccurate. Therefore, using Method-3 could have led to inaccurate surrogates if there was a discrepancy in the input values as described above. In addition, Method-1 predicted the hydrogen levels better than Method-3.

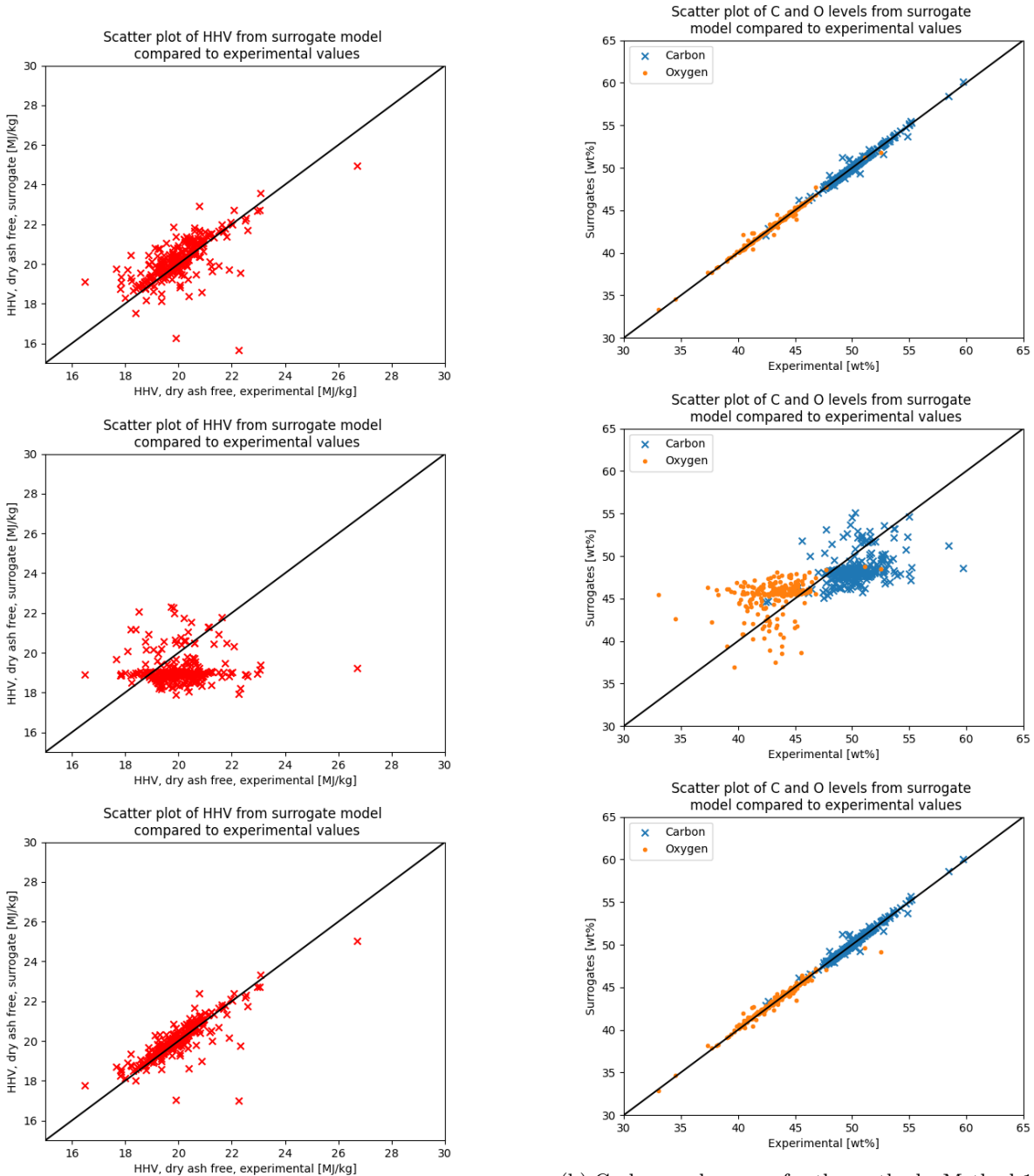
It must be noted that the best method was found using the waste component untreated wood, and therefore Method-1 is not necessarily the best method for all waste components. Still, untreated wood had the most data points available, which was a great benefit when deciding which method to use for the surrogate formulation.

Table 7: Average experimental values, and average values from each method

	C[wt%]	H[wt%]	O[wt%]	N[wt%]	S[wt%]	HHV[MJ/kg]
Experimental	50.320	6.089	43.217	0.284	0.048	20.003
Method 1	50.372	6.019	43.260	0.301	0.048	20.203
Method 2	48.513	5.859	45.298	0.283	0.046	19.155
Method 3	50.421	5.908	43.305	0.316	0.050	20.084

Table 8: Summary of how each method matched the data points' experimental values, good means that it matched the experimental values fairly well

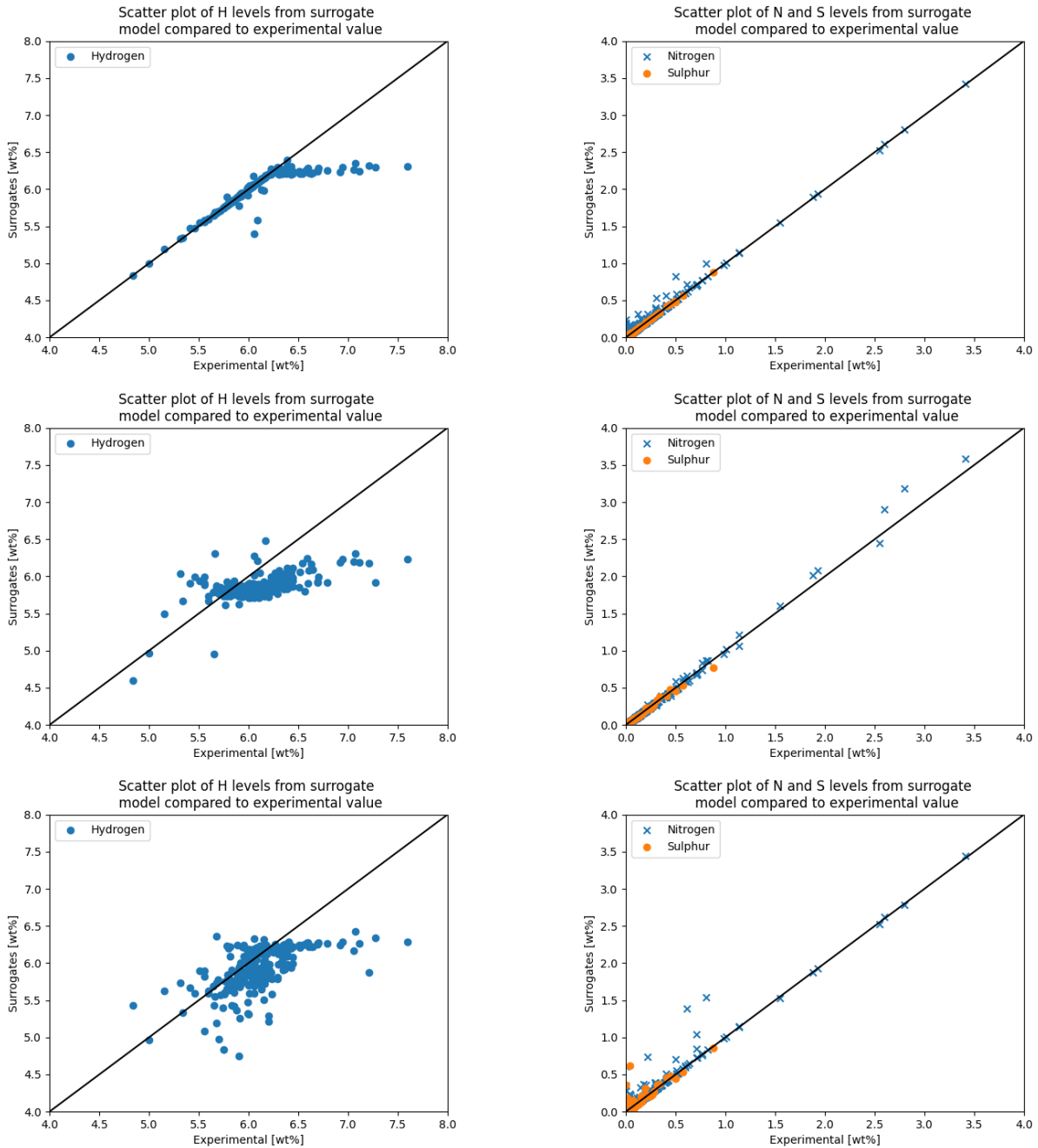
Method	C	H	O	N	S	HHV
Method 1	Good	Good, except data points with high H levels	Good	Good	Good	Good
Method 2	Underpredicted	Underpredicted	Overpredicted	Good	Good	Underpredicted
Method 3	Good	Underpredicted	Good	Overpredicted for some data points	Overpredicted for some data points	Good



(a) HHV for the methods, Method-1 is at the top, Method-2 in the middle, and Method-3 at the bottom

(b) Carbon and oxygen for the methods, Method-1 is at the top, Method-2 in the middle, and Method-3 at the bottom

Figure 9: Scatter plots of experimental values compared to the surrogates



(a) Hydrogen for the methods, Method-1 is at the top, Method-2 in the middle, and Method-3 at the bottom

(b) Nitrogen and sulphur for the methods, Method-1 is at the top, Method-2 in the middle, and Method-3 at the bottom

Figure 10: Scatter plots of experimental values compared to the surrogates

3.5 Formulating Surrogates for each Component

As described in the introduction, this thesis aimed to represent each waste class with surrogates. To do this, the steps from section 3.1 were used. In the process, it was found that three new surrogate species were needed, and these are described in section 3.6.

As explained in section 3.1, the formulation of the surrogates is thoroughly described for woody biomass. A summary of what was done is presented for the rest of the components, but the choices were based on an analysis similar to what was done for woody biomass.

3.5.1 Woody Biomass

The waste components belonging to the category of woody biomass are shown in Table 9 and were based on the categorisation done in section 3.2. The table also shows how many data points were available for each component [8].

Table 9: Components, their respective waste class and available data points

Component	Waste class	Data points	Component	Waste class	Data Points
Park Wood	1131	38	Leaves and needles	1131	7
Grass	1131	23	Untreated wood	1141	253
Treated wood	1142	41	Wood Chips	1143	88
Sawdust	1143	20	Bark	1143	42
Mixed treated wood	1149	14	Creosote-treated wood	7154	11
Textiles	1911 and 7022	5	Furniture wood	1912	11
CCA-treated wood	7098	11	Paper	1506, 7022 and 7024	51

The surrogate formulation and selection were based on untreated wood, and deviations for other components are explained. As in section 3.4.1, untreated wood was chosen since this component offers the most data points.

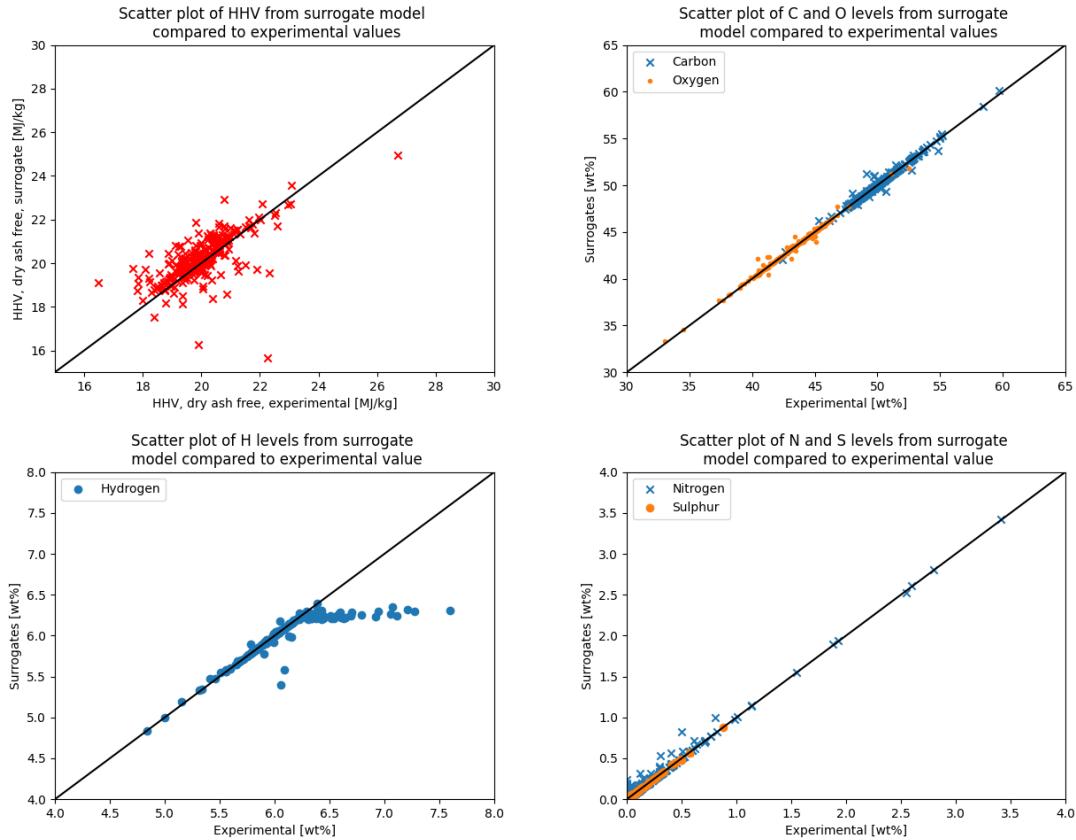


Figure 11: Scatter plot of the HHV, carbon, oxygen, hydrogen, nitrogen and sulphur levels from the experimental data compared to the surrogates

First, the surrogates were formulated using the surrogate species available in the MSW model by Netzer et al. [6], with the plastic species omitted. These surrogates were CELL, HCE, LIGC, LIGH, LIGO, PROT, NH₃i, CO₂i and sulphur explained in section 2.2. In addition, some surrogate species were merged as described in Equation 2 to 5. Using these gave the average elemental composition and higher heating value on the dry ash-free basis as seen in Table 10 and Figure 11. The average composition of the surrogate species can be found in Table 11, while Figure 12 shows the surrogate

species composition for the whole data set shown as a box plot. An explanation of how the box plot represents data can be found in section 2.4.

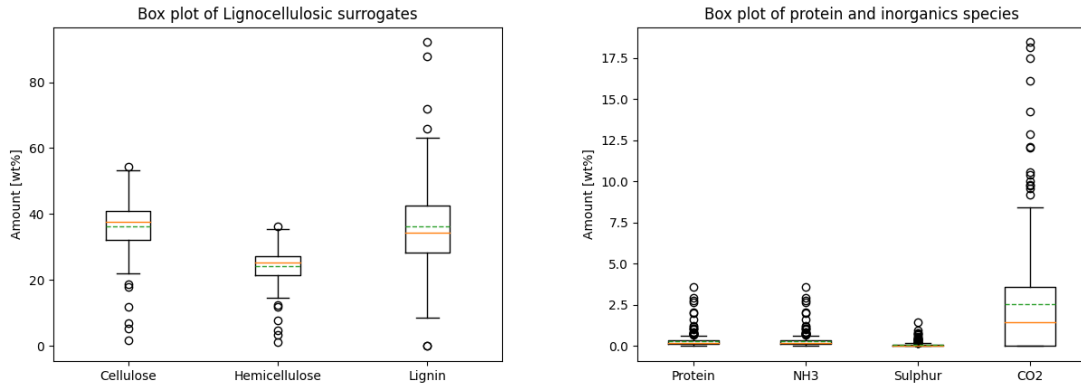


Figure 12: Box plot of the surrogate species used

Figure 11 shows that the surrogates matched the experimental HHV and elements for most data points. However, one can see that the surrogates underpredicted the hydrogen content for data points where the experimental content was above 6.5 wt%. This is due to the assignment seen in Figure 13, which shows the surrogate species used in a C-H plot. According to experiments, untreated wood should be composed of around 90% of lignocellulosic species [31], so most of the data points in Figure 13 should fall between the blue lines. As can be seen, this was not the case, and therefore surrogate species such as protein, NH_3 and CO_2 were assigned more than they should be for some data points, as can be seen in Figure 12. This was the reason for the disparity between the surrogates and experiments for hydrogen levels over 6%. In Figure 13, one can see that when the hydrogen level starts to go above 6.5%, the data can no longer be described by mostly using lignocellulosic species.

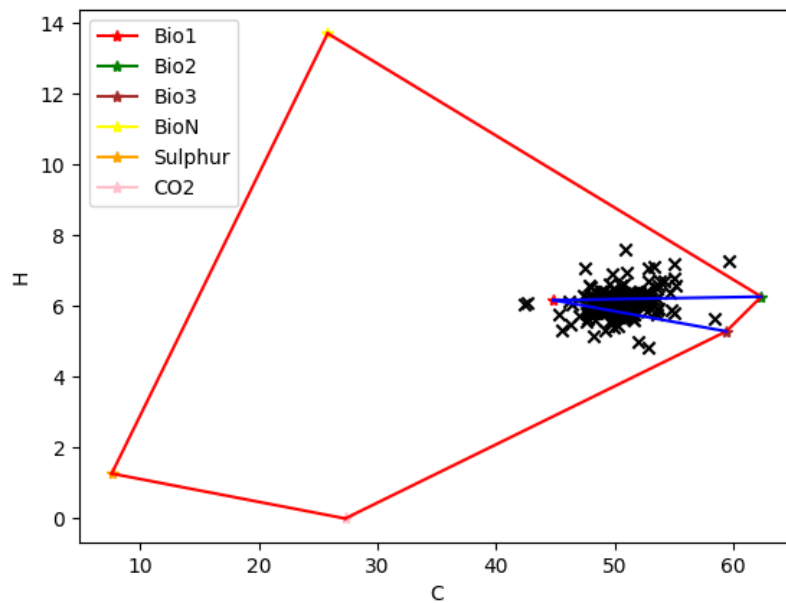


Figure 13: C-H plot of surrogate species used. The red line shows the area covered by all surrogate species. The blue line shows the area covered by the lignocellulosic species

A solution to this problem was to use a setup described by Debiagi et al. [31]. There, the surrogate species were assigned the same way as earlier, but they added the two species of tannin and triglycerides to Bio-2 and Bio-3. This allowed Bio-1, Bio-2 and Bio-3 to account for more of the surrogates. This seemed like the solution for improving the surrogate formulation. Since it was deemed favourable not to make more new surrogate species than necessary, the species tannin and triglycerides were substituted with surrogate species from the sewage sludge model by Netzer et al. [12]:

Tannin ($C_{15}H_{12}O_7$) was replaced with sugar ($C_6H_8O_6$): Since sugar is oxygen-rich like tannin, and a natural part of most plant-based material, although in limited amounts [41]. However, because the C/H/O ratio of sugar is not quite the same as tannin, the setup in this thesis differed a bit from the setup by Debiagi et al. [31].

Triglycerides ($C_{57}H_{100}O_7$) was replaced with lipid $C_{18}H_{32}O_2$: The lipid species is a general species created to cover fats and greases [11]. Since triglyceride is a type of lipid [42], and the C/H/O ratio of both species is almost equal, replacing it with lipid did most likely not affect the results compared to Debiagi et al. [31].

Based on Debiagi et al. [31] and Netzer et al. [12], the surrogate species were then merged into Bio-22 and Bio-33 seen in Equation 17 and 18. Bio-1 and Bio-n were left as in Equation 2 and 5.

$$\text{Bio-22} = 0.16 \cdot \text{LIGC} + 0.64 \cdot \text{LIGH} + 0.2 \cdot \text{LIPID} \quad (17)$$

$$\text{Bio-32} = 0.16 \cdot \text{LIGC} + 0.64 \cdot \text{LIGO} + 0.2 \cdot \text{SUGAR} \quad (18)$$

In addition to changing Bio-2 and Bio-3, it was decided not to use the inorganic carbon and nitrogen species. As seen in Figure 12, the amount of inorganic carbon was relatively high, especially for some data points, and in woody biomass, the amount of inorganic materials is generally negligible [41]. This also meant that the merged component Bio-n could not be used anymore, and PROT were set as an individual surrogate species in the model. The new setup gave the results shown in Table 19 and 20, and Figure 15 and 14.

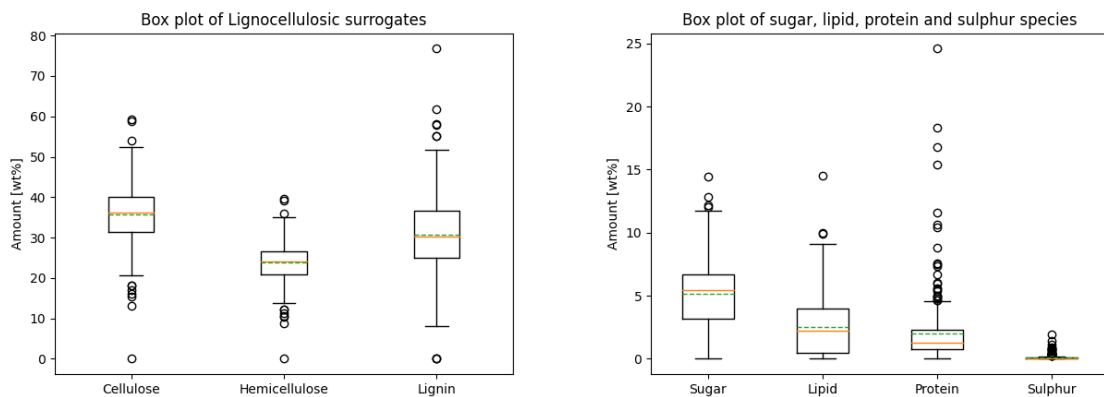


Figure 14: Box plot of the surrogate species used

As shown in Figure 15, the hydrogen level from the surrogates now matched the experimental values better than before. The HHV, C and O were about the same as the last method. However, the nitrogen and sulphur levels became somewhat incorrect, as seen in Figure 15. This was most likely due to the removal of the inorganic carbon and nitrogen, which alters the assignment of the surrogate species. Removing the inorganic nitrogen made PROT the only surrogate species accounting for the nitrogen, and the PROT species consisted of less nitrogen than the inorganic nitrogen. This might be the reason why the nitrogen was underpredicted. Removing inorganic

carbon and nitrogen led to some outliers for the sulphur, which was deemed acceptable since the component consists of 253 data points.

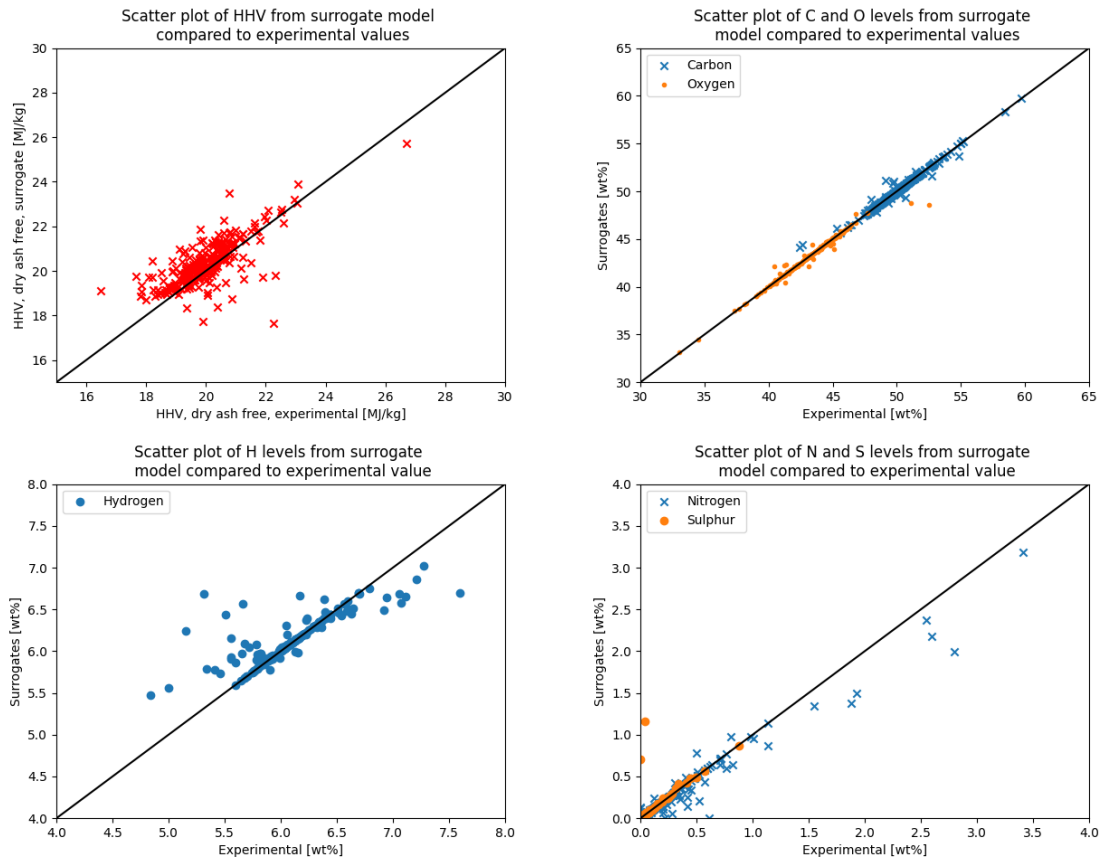


Figure 15: Scatter plot of the HHV, carbon, oxygen, hydrogen, nitrogen and sulphur from the experimental data compared to the surrogates

To make a surrogate formulation that matched the experimental values better, the PROT species was replaced by three different PROT species, as was done in the model for sewage sludge by Netzer et al. [12]. The three protein species were $PROT_C$, $PROT_H$ and $PROT_O$, as described in section 2.2. Three different protein species were believed to increase the accuracy for the surrogates since it led to more species being able to describe the nitrogen level. This setup gave the results shown in Table 10 and 11, and Figure 17 and 16

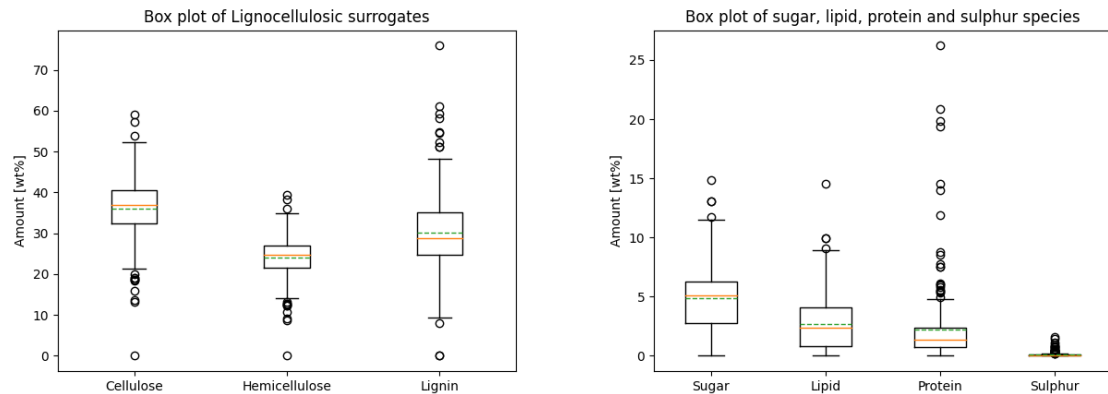


Figure 16: Box plot of the surrogates species used

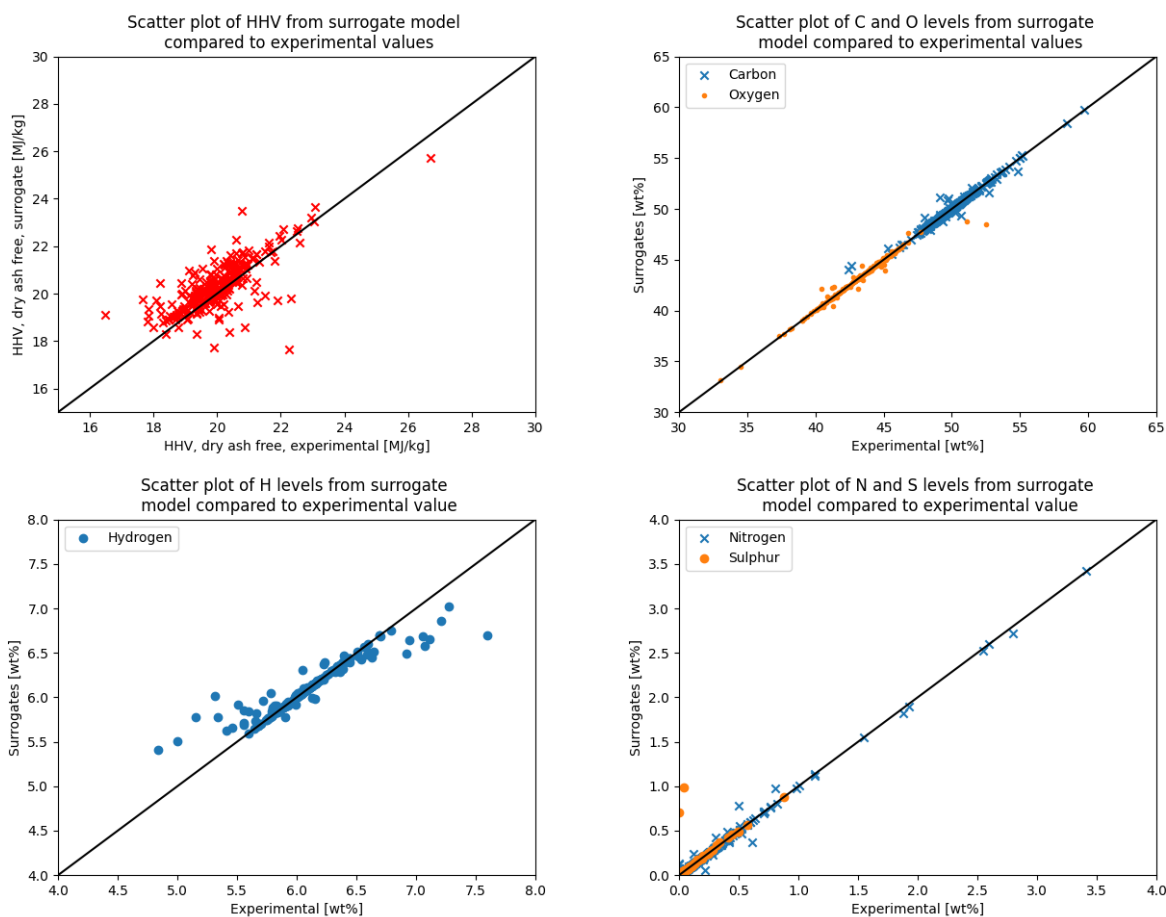


Figure 17: Scatter plot of the HHV, carbon, oxygen, hydrogen, nitrogen and sulphur from the experimental data compared to the surrogates

One can see that this surrogate formulation led to nitrogen and hydrogen levels that matched the experimental values better, while it was about the same as the last model regarding the remaining parameters. Therefore, it was decided that the last setup, setup 3, created the best surrogate formulation for the component untreated wood. The amount of each surrogate species used for the surrogates also seemed realistic. The amount of cellulose, hemicellulose and lignin found in wood is generally around 40-50%, 25-35% and 18-25%, respectively, while the extractives (sugar, lipid and protein) are generally around 4-10% [41]. In the last assignment, the values for cellulose, hemicellulose, lignin and extractives were around 36%, 24%, 30% and 10%, respectively, which was relatively close to these values.

One shortcoming of this surrogate formulation was that it did not include a surrogate species that accounts for the small amounts of chlorine in wood. This was because the surrogate species explained in 2.2 did not include any species containing chlorine other than PVC plastic. And since it would not be suitable to include a plastic species when explaining woody biomass, no species containing chlorine were available. The solution for this would have been to create a new surrogate species, as was done for some species in section 3.6. However, creating a chlorine species for the organic materials would be far more laborious than creating the species made in section 3.6 since no apparent real species could account for the chlorine in wood. Therefore, due to time constraints, it was not done in this thesis. Consequently, this thesis has no chlorine species for the organic materials. However, the chlorine level of most plant-based materials was minuscule, so it will not affect the model significantly. Nevertheless, as explained in the introduction, HCl and dioxins are often of interest when looking at emissions of a combustion process. These can be modelled incorrectly when the model has no chlorine surrogate species for organic materials.

Table 10: Average amount of elements from the experimental data and the different assignments

Source	C [wt%]	H [wt%]	O [wt%]	N [wt%]	S [wt%]	Cl [wt%]	HHV [MJ/kg]
Experimental	50.320	6.089	43.217	0.284	0.048	0.031	20.003
Setup 1	50.372	6.019	43.259	0.301	0.048	0	20.203
Setup 2	50.355	6.121	43.205	0.263	0.057	0	20.323
Setup 3	50.355	6.097	43.207	0.285	0.055	0	20.295

Table 11: Average amount of surrogate species used for each assignment in wt%

Source	CELL	HCE	LIG	PROT	SUGAR	LIPID	NH ₃ i	CO ₂ i	Sulphur
Setup 1	36.23	24.15	36.15	0.32	-	-	0.32	2.76	0.08
Setup 2	35.65	23.77	30.76	2.03	5.16	2.53	-	-	0.09
Setup 3	36.04	24.03	30.11	2.19	4.83	2.70	-	-	0.09

A setup for formulating the surrogate for the component untreated wood was found. This setup was assumed to work well for other woody biomass components. However, alterations were made to accommodate distinctive features seen in some components. The alterations made were the following:

Furniture Wood: It was found that the experimental values for furniture wood contained more nitrogen than the other wood components [38]. This was most likely due to additives used in creating furniture wood [43]. This led to the formulation using a disproportionate amount of the protein surrogate species. Therefore, it was decided that the surrogate formulation for furniture wood would include Bio-n as described in Equation 5 so that the inorganic nitrogen species were included.

Textiles: It was assumed that textiles primarily consist of cotton. Since cotton consists almost entirely of cellulose [44], Bio-1 was replaced with Bio-4, seen in Equation 19. It was also set a limit of 5% for Bio-2 and Bio-3 because cotton consists almost entirely of cellulose [44]. In addition, PET was added to the solution. This was done because some input values consisted of textiles derived from MSW [45, 46], and could therefore consist of both synthetic and plant-based textiles. PET was chosen since this is used in polyester, the most common synthetic textile [47]. PET plastic was one of the surrogate species created in this thesis, as seen in section 3.6. As for furniture wood, Bio-N accounted for nitrogen-rich additives that might be used when producing textiles.

$$\text{Bio-4} = 0.9 \cdot \text{CELL} + 0.1 \cdot \text{HCE} \quad (19)$$

Treated wood and mixed treated wood: Both mixed treated wood (e.g. plywood, particle wood) and treated wood (e.g. demolition wood) often consist of different non-biological materials, such as resins, glue and paint [43]. To account for this, it was chosen to use PET and PVC when formulating the surrogates for these two components. PET was chosen since it is a common plastic, and since it is a polymer with relatively high carbon and hydrogen content, it can account for the glue and paint contents. In addition, the resin used for many wood components contains oxygen [43], so the oxygen content in PET can account for this. Adding PVC to the surrogates made it possible to model the chlorine level of the components, something that was not possible for the other woody biomass components. As for furniture-wood and textiles, bio-N accounted for additives rich in nitrogen.

Creosote-treated Wood: Creosote is derived from distilling tar from wood or coal [48]. To model this component, the new surrogate species asphaltene, created in section 3.6, was used to account for the creosote. In addition, it was chosen to make asphaltene account for the nitrogen in the component. This was done because formulating the surrogates with the proteins included produced inaccurate results. This was probably because the asphaltene species contained nitrogen, and including this in addition to the protein miscalculated the amount of nitrogen. Therefore, the protein species were removed, even though this component, like the other wood components, would likely contain some protein.

Paper: Paper mostly consists of cellulose [49]. Therefore, it was decided to change Bio-1 to account for more cellulose content. The new Bio-5 can be seen in Equation 20. Also, sugar and lipid were not used for paper. This was because sugar and lipid were added to account for wood extractives. However, paper does not generally contain these extractives since these are most often removed in the manufacturing process [50]. Therefore, Bio-2 and Bio-3, as seen in Equation 3 and 4 were used. Inorganic carbon and nitrogen were added to account for additives used in paper that might contain nitrogen or carbon [51]. PE and PVC were added for the same reason since paper can often contain some polymers [51]. Adding the PVC also made it possible to model the chlorine content.

$$\text{Bio-5} = 0.8 \cdot \text{CELL} + 0.2 \cdot \text{HCE} \quad (20)$$

The ultimate analysis, heating value and surrogate species composition from the surrogates of woody biomass can be found in section 4.1.

3.5.2 Sludge and other Biomass

The waste components in the sludge and other biomass category are shown in Table 12 and were based on the categorisation done in section 3.2. The table also shows how many data points were available for each component [8].

Table 12: Components and their respective waste class and available data points

Component	Part of waste class	Data points	Component	Part of Waste class	Data points
Sewage sludge	1126	17	Organic domestic waste	1111	15
Paper Sludge	1126	8	Leather	1911	5

Since this waste category only contained four components, compared to the 14 components of woody biomass, it was decided to find a surrogate formulation for each component.

Sewage sludge and Organic domestic waste: For sewage sludge, the surrogate species from the model by Netzer et al. regarding sewage sludge were used [12]. In this article the component Bio-1, Bio-6 and Bio-7, as seen in Equation 2, 21 and 22 were used. The rest of the surrogate species used were SUGAR, LIPID, $PROT_H$, $PROT_O$, $PROT_C$, NH_{3i} , CO_{2i} and sulphur, which are explained in section 2.2. This means that, unlike woody biomass, sugar and lipid were surrogate species on their own.

$$\text{Bio-6} = 0.95 \cdot \text{LIG}_O + 0.05 \cdot \text{LIG}_C \quad (21)$$

$$\text{Bio-7} = 0.95 \cdot \text{LIG}_H + 0.05 \cdot \text{LIG}_C \quad (22)$$

This model created decent results compared to the experimental values for sewage sludge. Still, as for woody biomass, no chlorine species were available for chlorine found in biomass. One way to include chlorine in the surrogates was to include PVC as a surrogate species, and this was done here. Although a chlorine species for biomass could create a more accurate surrogate formulation, PVC was still a viable option. Sewage sludge often contains small amounts of plastics, especially microplastics [52], so using a plastic species is realistic. It was also found that the setup worked well for the component organic domestic waste.

Leather: The setup used for sewage sludge and organic domestic waste was used with a couple of changes for leather. First, Bio-1, Bio-6, Bio-7 and sugar were removed. This was because leather contains no plant-based materials and is therefore described using mostly lipid and protein. The inorganic carbon and nitrogen were included to account for any inorganics present, especially from

the manufacturing process [53]. However, including inorganic carbon led to inaccurate results, so it was decided to only use inorganic nitrogen to account for the additives. Leather might also contain some chlorine, and it was deemed acceptable to use PVC as a surrogate species to account for the chlorine, since processed leather might contain small parts of polymers [53].

Paper Sludge: It was assumed that paper sludge had about the same composition as paper, and could be described using the same setup as was done for paper in section 3.5.1.

The results from the waste components in this category can be found in section 4.2.

3.5.3 Mixed Waste

The waste components belonging to the category of mixed waste are shown in Table 13 and were based on the categorisation done in section 3.2. The table also shows how many data points were available for each component [8].

Table 13: Components, their respective waste class and available data points

Component	Part of waste class	Data points
Hospital waste	6004	5
Municipal solid waste	9911	22
Refuse-derived fuel	9913	30

The MSW component was used to find a setup for the mixed waste components. First, the surrogates was formulated using the surrogate species from the model regarding MSW by Netzer et al. [6], which can be found in section 2.2. These species gave adequate results, with all the elements being modelled fairly well compared to the experimental values. The HHV was inaccurate for some of the values compared to the experimental values. Also, the amount of inorganic carbon seemed overpredicted [38].

In order to model MSW more accurately, a couple of changes were made to the formulation. First, sugar and lipid were added as new species. This was done to account for the organic domestic waste often found in MSW [54]. Bio-n was also removed, and the protein and inorganic nitrogen were therefore modelled individually, with the protein being modelled using the three protein species $PROT_C$, $PROT_H$, $PROT_O$ from the sewage sludge model by Netzer et al. [12] and the inorganic nitrogen by using the species NH_3i . The inorganic nitrogen and carbon were limited by the ash content, as was done in a model by Debiagi et al. [11]. Lastly, two of the surrogates species created in section 3.6 were added, PET and natural rubber (NR). PET was added to model the plastics found in municipal solid waste more accurately, while NR was added to account for the rubber often found in MSW [55, 56].

Refuse-derived Fuel: Refuse-derived fuel (RDF) is waste that has been sorted, crashed, and pelletised [57]. This usually means most metals and glass have been removed from the waste. Since removing metal and glass does not affect the surrogate formulation (it is modelled without ash), it was assumed that RDF could be modelled using the same setup as MSW.

Hospital Waste: As explained in the project work [8], this waste class consists of non-infectious waste from hospitals. Therefore, it was found fair to assume that this waste class mostly contains the same as MSW, with the differences being picked up by the model itself.

The results from the waste components in this category can be found in section 4.3.

3.5.4 Rubber Waste

The waste components belonging to the category of rubber waste are shown in Table 14 and were based on the categorisation done in section 3.2. The table also shows how many data points were

available for each component [8].

Table 14: Components, their respective waste class and available data points

Component	Part of waste class	Data points	Component	Part of waste class	Data points
Passenger Tyres	1811	13	Truck Tyres	1812	9
MC/Bike tyres	1814	7	Rubber Waste	1899	9

To find surrogates for the rubber waste components, it was set up using the passenger tyre component. Since different types of tyres contain mostly the same materials, only with varying ratios of the materials, it was assumed that the setup used for passenger tyres could be used for all the components [58].

First, the surrogates was set up using the species from the MSW model by Netzer et al. [6], with the organic materials removed [58]. The model did not have any rubber surrogate species, but it did contain PS, which is a polymer of styrene [26]. Therefore, it was assumed that it was an adequate surrogate species for the synthetic rubber styrene-butadiene, which is widely used in tyres [59]. Using these surrogate species gave adequate results, but it gave high amounts of the PS surrogate species. This was because the surrogates did not include natural rubber, an often essential part of tyres [58]. Therefore, a new surrogate species called natural rubber (NR) was created and added to the surrogate formulation. PET and PA were also included since the textiles used in car tyres are often made from polyester or nylon [58, 60], which can be accounted for by using PET and PA. The results from the surrogates can be found in section 4.4.

3.5.5 Plastics

The waste components belonging to the category of plastics are shown in Table 15 and were based on the categorisation done in section 3.2. The table also shows how many data points were available for each component [8].

Table 15: Components, their respective waste class and available data points

Component	Part of waste class	Data points	Component	Part of Waste class	Data points
Cables	1504	5	PVC	1506	5
PP	1506	5	PE	1506	5
PS	1506	5	PET	1506	5
Glass fibre plastics	1751, 2431	3	Synthetic textiles	1911	3
Carbon fibre plastics	1751	2			

For this category, no specific component was used to find the surrogate formulation. There were two reasons for this. Firstly, this category’s components are quite different. The second reason is that many of these components could be found as surrogate species on their own. PP, PS, PVC and PE were all available from the surrogate species described in section 2.2, while PET was described using the surrogate species PET created in section 3.6

The setup for formulating the surrogates for the pure plastic components was to use the corresponding surrogate species available from section 2.2, as well as the new PET surrogate species created in section 3.6.

Glass and carbon fibre-reinforced plastic is made of glass or carbon fibre with a polymer. In the author’s project work [8], two of the data points for glass and carbon fibre were described as a mix of these two. These were not included in any of the surrogates for simplicity.

Cables are generally made up of different plastics. Synthetic textiles are also made of plastics, especially PE and PA [61]. Therefore, all the plastic species from section 2.2, the inorganic nitrogen and carbon, and the sulphur species were included in the surrogates for carbon and glass fibre,

cables and synthetic textiles. In addition, as was done in a model by Debiagi et al. [11], each data point’s ash content limited the inorganic carbon and nitrogen since these values would otherwise become quite large. The PET surrogate species created in section 3.6 was also included. Using these surrogate species to formulate the surrogates produced the results in section 4.5.

3.5.6 Oil-based Waste

The waste components belonging to the category of oil-based wastes are shown in Table 16, and were based on the categorisation done in section 3.2. The table also shows how many data points were available for each component [8].

Table 16: Components, their respective waste class and available data points

Component	Part of waste class	Data points	Component	Part of Waste class	Data points
Asphalt	1621	3	Diesel	7142	4
Oil cuttings	7143	5	Distillation residue	7152	4
Tar	7152	3	Activated carbon	7152	4
Oil	7021, 7022, 7024	8			

The oil-based waste components had some variations regarding their composition. Therefore it was not found a setup for one of the components to be used for all. Furthermore, it was observed that these components could not be made using the surrogate species from the MSW or sewage sludge model by Netzer et al. [6, 12]. Therefore, the surrogate species asphaltene was created to model these components. The surrogates of the components of this category were found using the following setup:

Asphalt: Asphalt contains considerable amounts of asphaltene [62], so the surrogate species asphaltene was used. Asphaltene does not include sulphur, so the sulphur species was added. The inorganic carbon and nitrogen species were added to model inorganic carbon and nitrogen that might be present in asphalt.

Oil and Oil cuttings: Oil-1, seen in Equation 23, was created to model oil since only using asphaltene provided inaccurate results. This was probably because oil contains lighter hydrocarbons in addition to asphaltene [63]. Therefore, the PE surrogate species was added to model the lighter hydrocarbons. This is not entirely realistic, but it was found adequate for formulating the surrogates. As for asphaltene, sulphur and inorganic carbon and nitrogen were used to formulate the surrogates. Oil cuttings were modelled the same way as oil since it was assumed that oil cuttings were oil and inorganic materials (ash).

$$\text{Oil-1} = 0.6 \cdot \text{PE} + 0.4 \cdot \text{ASPH} \quad (23)$$

Diesel: Diesel was set up in almost the same way as oil, but Oil-1 were replaced with Oil-2, seen in Equation 24. This was done since diesel is composed of lighter hydrocarbons than oil [64]. Therefore, the surrogates became more accurate with a higher content of PE. However, setting it to only PE instead of including some asphaltene gave more inaccurate results than the ratio in Oil-2. Therefore, Oil-2 was used in addition to sulphur and inorganic carbon and nitrogen.

$$\text{Oil-2} = 0.95 \cdot \text{PE} + 0.05 \cdot \text{ASPH} \quad (24)$$

Distillation residue: This component was set up similarly to asphalt. The reason for formulating is similarly to asphalt is that it was assumed that distillation residue consisted of heavy hydrocarbons. Therefore this setup used asphaltene, sulphur and inorganic nitrogen and carbon.

Tar: Tar was set up similarly to oil. However, it was found that using Oil-1 provided inaccurate results. Therefore, Oil-1 was replaced with Oil-3, which provided results closer to the experimental

values. This might indicate that the component tar contains heavier hydrocarbons than the oil component. Everything in the setup was the same as for oil, except for the different oil component.

$$\text{Oil-3} = 0.15 \cdot \text{PE} + 0.85 \cdot \text{ASPH} \quad (25)$$

Activated Carbon: Modelling activated carbon using the surrogate species available gave unsatisfactory results. This is due to the high carbon content, which no existing surrogate species had. Therefore, the plastic species PS was used since this provided the highest carbon level of the surrogate species. This is not entirely correct, but it was found acceptable for modelling the activated carbon. Therefore, the species used were PS, asphaltene, sulphur and inorganic carbon and nitrogen.

3.6 New Surrogate Species

It was found that three surrogate species were missing to create surrogates for all components:

- **Natural Rubber:** Natural rubber is often a central component of tyres and other rubber waste [58]. In addition, it can be found in the mixed waste components since they often contain some rubber waste [55, 56]. However, natural rubber is not the only type of rubber, and in the literature, one finds that most rubber waste consists of a mix of several different rubbers [65]. The reason for only creating natural rubber is due to time constraints, as creating several different rubber types would have been too laborious. Nevertheless, it might be that only using natural rubber predicts the properties of the rubber waste well enough. Also, one of the synthetic rubbers often used is styrene-butadiene rubber, a polymer of styrene and butadiene [59]. The available surrogate species PS is a polymer of styrene, and therefore it was assumed that it could adequately model the synthetic rubbers.
- **PET:** PET was added to model plastics with high oxygen content. The components MSW, RDF and synthetic textiles were examples of waste components that typically contain some amounts of PET, and one of the components in this thesis was pure PET.
- **Asphaltene:** Asphaltene was added to describe oil-based waste components (not plastics). Asphaltene was chosen as a new surrogate species since its composition and properties, described further in section 3.6.4, was believed to model oil well. However, it was discovered that a lighter hydrocarbon was needed to model components such as oil correctly. In this thesis, this was solved by using PE for the lighter hydrocarbons.

The surrogate species were created using the following steps:

1. Create a reaction for the surrogate species based on experiments. The reaction was created based on the following criteria, where number 1 was decided to be the most important, while number 4 was the least important:
 - 1. Elemental balance: The stoichiometric balance for the reaction had to be balanced.
 - 2. Gas/oil/char balance: The amount of gas, oil and char in the products should be based on the amounts found in experiments.
 - 3. Consistency of the gas phase chemistry: Only react to species that already exist within the system: The products in the reaction should only consist of species found in the database [6]. This is because the model also includes the continued reaction of the products, and therefore the reaction and reaction rates of the products are needed. The group contribution method could be used if a species was needed but unavailable in the database. This is a method where large molecules can be described using different functional groups.
 - 4. The ratio of released aromatics/olefins/alkanes etc.: The tar composition of the products can be based on the amounts found in experiments.

-
2. Find relevant kinetic parameters for the reaction from experiments or other relevant literature. These parameters describe the Arrhenius Equation [30], namely the frequency, A , and the activation energy, E_a .
 3. Simulate the reaction using a stochastic reactor model in LOGEResearch using the setup explained in section 3.6.1. This was done to create a thermogravimetric graph of the surrogates' pyrolysis, which could then be compared to experimental data.
 4. If the reaction matches the experimental data, the surrogate species can be added to the model.

The process for each surrogate species can be found below, where section 3.6.2 explains the process for natural rubber, section 3.6.3 for PET and section 3.6.4 for asphaltene.

3.6.1 LOGEResearch Setup

A stochastic reactor model, as described in section 2.3, was used to simulate the reaction for the new surrogate species. The model was set up in LOGEResearch version 1.10 [66]. The setup was the same as used by Netzer et al. [6] and is a typical thermogravimetric (TG) analysis setup, with 272 species and 3885 reactions.

The reaction mechanism used already contained the reaction of numerous species [6]. These were needed since the model simulates the pyrolysis of the surrogates species and therefore models the products' continued reaction after the initial reaction. Adding new surrogate species into the model was done by adding the species' reaction, kinetic parameters, and elemental composition. The model setup can be found in appendix B.

In order to validate the setup, it was tested with the pyrolysis of PE and compared against the results produced by Netzer et al. [6]. The result is presented in Figure 18, and it can be seen that the setup matched the model and could therefore be used for modelling the new surrogate species.

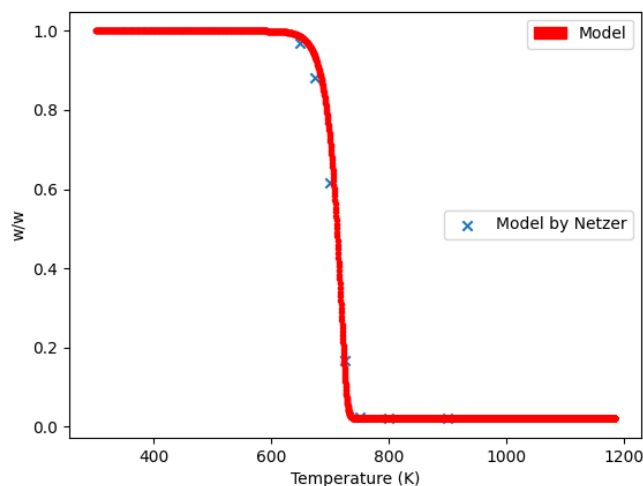


Figure 18: TG curves for the pyrolysis of PE. The red line is the result from this thesis. The marks show the results from the model by Netzer et al. [6]

3.6.2 Natural Rubber

The steps explained at the start of the section were used when creating the reaction for natural rubber. First, it was found that natural rubber can be modelled as cis-1,4-polyisoprene, which has

the chemical formula $[C_5H_8]_n$ [67]. This is a polymer, so it was decided to use a n-value of five as for the other polymer surrogate species in the model. Therefore, natural rubber was modelled as $[C_5H_8]_5$. Next, two articles regarding the amount of gas, tar and char were found [68, 69], where one of these contained information regarding the composition of the tar produced [69]. These articles provided ranges for how much gas, tar and char could be in the products, as well as an indication of how much aliphates, small aromatics and large aromatics the tar consists of. These char, tar and gas values are shown in Table 17. It was decided to use IC_5H_{10} to model the aliphates, C_6H_6 to model the small aromatics and $C_{10}H_8$ to model the large aromatics. CH_4 and C_2H_4 were used to model the gas products, and H_2 and $G(H_2)$ was added in order to balance the hydrogen. Where $G(H_2)$ is H_2 trapped in the solid. $C(S)$ was used to model the char in the reaction.

Table 17: Amount of gas, char and tar in natural rubber pyrolysis products [68, 69]

	Min [wt%]	Max [wt%]
Gas	2.1	4.3
Char	0	1.3
Tar	95.7	96.6

The natural rubber's kinetic parameters were $6.485 \cdot 10^{14} s^{-1}$ for the frequency and 207 kJ/mol for the activation energy [70]. The product species and information regarding the gas, char and tar were used to create a sufficient reaction. Each reaction was tested in the same LOGEResearch setup as PE, with the abovementioned kinetic parameters, and compared to experimental pyrolysis thermogravimetric data [69, 71, 72, 73]. The reaction was altered until a reaction that met the char, gas, and tar (and tar content) criteria matched the experimental data was found. The final reaction, shown in Equation 26, predicted the thermogravimetric graph seen in Figure 19, and it can be seen that the model matched the experiments well.

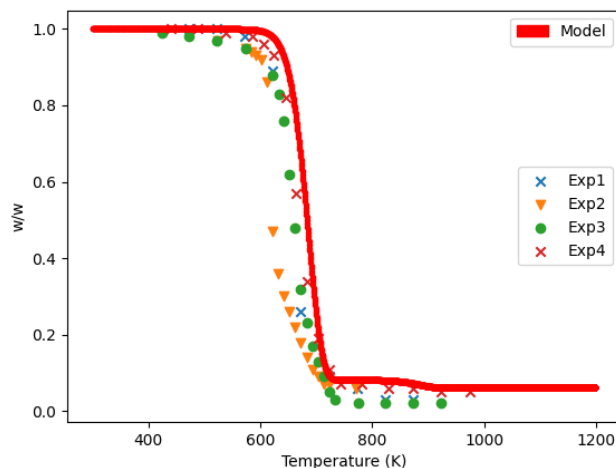
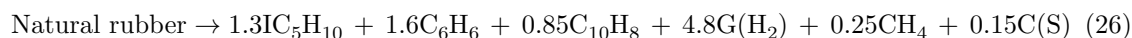


Figure 19: TG curves for the pyrolysis of NR. The red line is the result from the reaction shown in Equation 26. The marks show the results from four experiments [69, 71, 72, 73].

3.6.3 PET

When creating the reaction for PET, the steps explained at the start of the section were used. It was found that PET can be described using the chemical formula $[C_{10}H_8O_4]_n$ [74]. This is a

polymer, and as for the others, an n-value of five was used. The chemical formula then became $[C_{10}H_8O_4]_5$. The amount of gas, tar and char were found in experiments by Çit et al. [75]. As for natural rubber, it provided ranges for the products' gas, char and tar content as seen in Table 18. Previous experiments found that the tar produced from the pyrolysis of PET contained significant amounts of benzoic acid [76]. However, the database did not contain benzoic acid [6]. Therefore, the group contribution method was used. It was assumed that benzoic acid with the chemical formula C_6H_5COOH [77] could be modelled using benzene (C_6H_6), a species with an alcohol group and a species with a carbonyl group, $C=O$. Here, the molecule with an alcohol group was decided to be C_2H_5OH , and the molecule with a carbonyl group was decided to be Methyl tert-butyl ether. Previous experiments also showed that the pyrolysis products contained some amounts of NaOH-soluble components [76]. It was decided to use IC_5H_{10} to model lighter hydrocarbons in the tar, C_6H_6 , C_2H_5OH and Methyl tert-butyl ether to model benzoic acid and C_2H_5OH to model the NaOH-soluble components. CH_4 , H_2 , CH_2CO , CO , $G(CO)$ and CO_2 was used to model the gas products, where $G(CO)$ was CO trapped inside the solid. $C(S)$ was used to model the char in the reaction.

The kinetic parameters for PET were found to be $2.565 \cdot 10^{13} s^{-1}$ for the frequency and 207.5 kJ/mol for the activation energy [78]. A sufficient reaction was created using the product species and information regarding the gas, char and tar. Each reaction was tested in the same LOGEResearch setup as PE, with the abovementioned kinetic parameters, and compared to experimental pyrolysis thermogravimetric data [79, 80]. The reaction was altered until a reaction that both met the criteria regarding char, gas, tar (and tar content) and matched the experimental data was found. The final reaction, shown in Equation 27, predicted the thermogravimetric graph seen in Figure 20, and it can be seen that the model matched the experiments well.

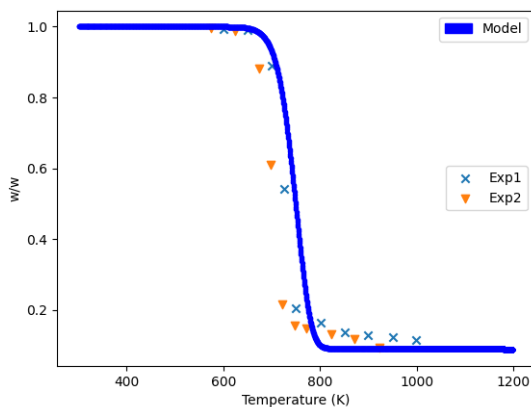
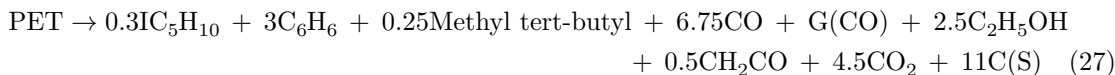


Figure 20: TG curves for the pyrolysis of PET. The blue line is the result from the reaction shown in Equation 27. The marks show the results from two experiments [79, 80].

Table 18: Amount of gas, char and tar in PET pyrolysis products [75]

	Min [wt%]	Max [wt%]
Gas	25	37
Char	8	17
Tar	46	64

3.6.4 Asphaltene

Contrary to PET and natural rubber, asphaltene does not have a clear-cut chemical formula, and its content can vary significantly depending on the sample [81]. However, Speight and Moschopedis provided a chemical formula that models asphaltene using $[C_{79}H_{92}N_2S_2O]_3$ [82]. However, using this formula in the LOGEResearch setup proved difficult since it contained too many elements. The solution to this problem was to remove the sulphur from the chemical formula and then use the sulphur species already provided when creating the surrogates for components containing asphaltene. Therefore, the chemical formula used here was $[C_{79}H_{92}N_2O]_3$. No direct limits for the gas, tar and char were used when setting up the reaction for asphaltene, but from pyrolysis experiments it was found that the products contained high amounts of char and a gas content generally around 10% [83, 84]. For asphaltene, C_5H_5N was used to model tar containing nitrogen, while $C_{10}H_8$ was used to model the tar not containing nitrogen. H_2 , $G(H_2)$, CH_4 , C_3H_8 and CO were used to model the gas, where $G(H_2)$ describes the gas trapped inside the solid. $C(S)$ was used to model the char.

The kinetic parameters for asphaltene were found based on a model by Guida et al. [85], where they had modelled asphaltene using five surrogate species. The kinetic parameters used in this thesis were created by taking the average of the kinetic parameters for these five surrogate species. Then, the frequency was found to be $1.02 \cdot 10^{13} s^{-1}$, and the activation energy 200.2 kJ/mol. The kinetic parameters and the elements described above were used to find the reaction for asphaltene. Each reaction was tested using LOGEResearch, with the same setup as PE. The reaction for asphaltene can be seen in Equation 28. Figure 21 shows how the reaction predicted the thermogravimetric graph compared to pyrolysis experiments [84, 86], and it can be seen that the reaction matched the experiments well.

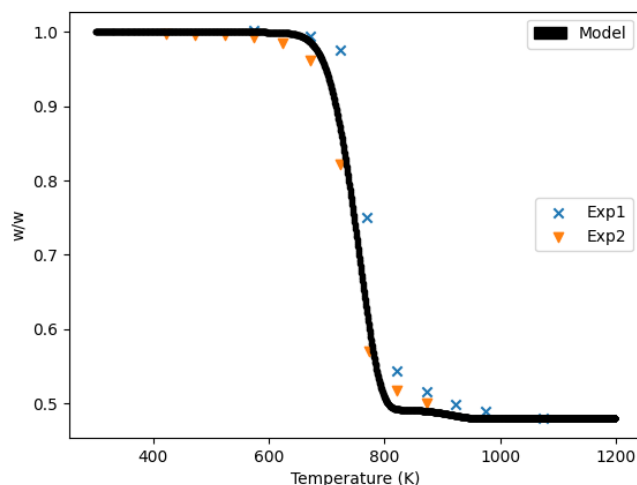
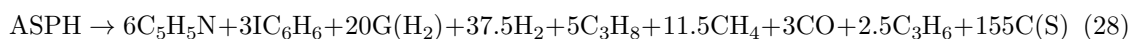


Figure 21: TG curves for the pyrolysis of Asphaltene. The black line is the result from the reaction shown in Equation 28. The marks show the results from two experiments [84, 86].

4 Results and Discussion

The surrogates of the components were created as described in section 3. The results presented here show the average value of their ultimate analysis and heating value and their relative error compared to the experimental values. It was decided that a relative error of 10% or less was acceptable, and only relative errors higher than this are discussed. The average composition of surrogate species for each component is also presented. The Excel files, scatter plots, and box plots that present the results in more detail can be found in a database [38].

In addition to the results for each component, a box plot, explained in section 2.4, of the HHV, N, S and Cl levels from the surrogates compared to the experimental values is presented. These four values were chosen because the HHV indicates how much energy the waste class contains, and is directly correlated to the C, H and O contents [40]. The sulphur, nitrogen and chlorine levels are important when considering the emissions generated. As explained in the introduction, NO_x, SO_x, HCl, and dioxins are especially troublesome emissions produced when incinerating waste.

Waste classes consisting of several components were not presented by a box plot. Instead, their average, maximum and minimum values are given. The maximum and minimum values were created by adding the components' highest and lowest data points. For example, if a waste class consisted of 40% of component 1 and 60% of component 2, then the maximum value would be

$$\text{Maximum} = 0.4 \cdot \text{Maximum of component 1} + 0.6 \cdot \text{maximum of component 2} \quad (29)$$

The same was done for the minimum. The average presented with the maximum and minimum indicates how heterogeneous the data is when the box plot is not used. For all the box plots and plots with average, maximum and minimum, values of zero were not included. This was because a value of zero often indicates that no value for this element was available, as explained in section 3.3.

4.1 Woody Biomass

The average ultimate analysis and HHV for each component from the surrogates are summarised in Table 19. The table also presents the relative error compared to the experimental data. Finally, Table 20 shows the average mass concentration of the surrogate species used in the surrogate formulation.

Table 19 shows that the surrogates for all components primarily produced results with less than 10% relative error for the ultimate analysis and HHV. The relative error of sulphur was larger than 10% for untreated wood, grass and CCA-treated wood. However, this was considered to be due to the low content of sulphur, which meant that minor absolute errors led to fairly large relative errors. The chlorine could not be modelled for the components, except the ones where the PVC surrogate species was used. The relative error for nitrogen was larger than 10% for creosote-treated wood, which was most likely because it was modelled with asphaltene and without protein. Using another surrogate species than asphaltene to account for the creosote might have improved the results for this component.

Figure 20 shows that the components made of wood (untreated wood, wood chips, sawdust, furniture wood, CCA-treated wood, park wood, treated wood, mixed treated wood and creosote-treated wood) had around the same amount of lignocellulosic surrogate species, with cellulose being 30-40%, hemicellulose 20-25%, lignin 30-35% and extractives (sugar, lipid and protein) being around 10%. These values were within what can be expected for wood [41]. Treated wood and mixed treated wood had different values for their lignocellulosic surrogate species, but this was because PET was used when modelling these. Especially the lignin values were different because using PET, which is carbon and hydrogen-rich, replaced some of the lignin used in the model.

Table 19: Overview of the elemental composition of the surrogates for the woody biomass. The upper row for each component shows the amount of the elements in wt%, and the HHV in MJ/kg. The lower row shows the relative error in % compared to the experimental values

Source	C	H	O	N	S	Cl	HHV
Untreated Wood	50.355	6.097	43.207	0.285	0.055	0	20.295
	0.07	0.13	0.02	0.35	14.58	100	1.46
Wood Chips	50.886	6.143	42.526	0.396	0.048	0	20.603
	0.16	0.47	0.14	3.66	0.0	100	2.17
Bark	53.264	5.925	40.443	0.326	0.041	0	21.392
	0.10	0.32	0.13	0.61	2.50	100	1.87
Sawdust	51.004	6.149	42.491	0.337	0.019	0	20.652
	0.16	0.18	0.19	0.59	0.0	100	2.04
Grass	49.468	6.143	41.941	2.170	0.277	0	20.165
	0.27	0.59	0.18	0.14	13.06	100	1.14
Furniture Wood	49.259	6.194	42.568	1.888	0.091	0	20.074
	1.32	0.03	1.43	2.33	0	100	0.82
CCA treated Wood	49.546	6.132	43.953	0.304	0.065	0	19.978
	0.14	1.41	0.03	4.83	14.04	100	0.01
Park Wood	50.234	5.996	42.933	0.773	0.063	0	20.156
	0.06	1.13	0	0.90	3.28	100	1.08
Leaves and Needles	51.169	6.190	41.099	1.401	0.141	0	20.899
	0.82	1.35	0.83	0.21	1.40	100	2.53
Textiles	51.534	5.749	40.983	1.526	0.208	0	20.525
	0.34	6.97	0.46	8.69	7.96	100	5.80
Demolition wood	51.165	6.111	41.722	0.863	0.069	0.070	20.741
	0.20	1.32	0.19	2.74	1.43	4.11	1.29
Treated wood	51.006	6.099	40.177	2.551	0.052	0.116	20.803
	0.02	0.86	0.04	0.58	4.00	2.52	5.35
Creosote-treated wood	53.994	6.175	39.507	0.209	0.114	0	22.049
	0.66	1.10	0.42	13.99	0.88	100	5.34
Paper	51.984	7.048	40.536	0.318	0.083	0.031	22.264
	0.01	0.01	0.01	0.0	0.0	8.82	1.56

Looking at the extractives for the components made of wood shows that they all had around the same amount of protein, sugar and lipid. Park wood had higher sugar content because this waste class contains smaller trees and trimmings, which often contain more extractives [87].

The surrogates for the rest of the components also looked realistic. Bark was described using large amounts of lignin and sugar compared to untreated wood since bark generally contains fair amounts of lignin and extractives [88]. Grass was described using considerable amounts of protein, corresponding with the amounts generally found in grass [89]. The textile component contained large amounts of cellulose and a small amount of hemicellulose and lignin, which is typical for cotton [44]. The large amount of PET is probably because it was synthetic materials in the data points since some of the input data were textiles from MSW [38]. Paper contained about 50% cellulose, which should have been higher since paper primarily consists of cellulose [49]. Also, the PE added to account for additives seems too high at 18%. The inorganic carbon was at 10%, which might represent the ink used in paper [90]. The inorganic carbon might also be relatively high because of the amount of PE used. Since the PE species do not contain oxygen, the inorganic carbon might have been assigned to balance the oxygen.

Table 20: Composition of surrogate species in wt% for woody biomass

Source	CELL	HCE	LIG	PROT	SUGAR	LIPID	NH ₃ i	Sulphur	Other
Untreated Wood	36.04	24.03	30.11	2.19	4.83	2.70	-	0.09	-
Wood Chips	34.70	23.13	31.23	3.05	4.68	3.12	-	0.08	-
Bark	21.89	14.60	48.75	2.51	8.92	3.27	-	0.07	-
Sawdust	34.07	22.71	32.48	2.59	4.77	3.35	-	0.03	-
Grass	29.28	19.52	27.26	16.67	5.45	1.37	-	0.46	-
Furniture Wood	32.54	21.69	33.32	1.98	6.90	1.43	1.98	0.15	-
CCA treated Wood	40.03	26.69	24.67	2.33	3.82	2.34	-	0.11	-
Park Wood	32.28	21.52	32.12	5.95	6.54	1.48	-	0.10	-
Leaves and Needles	28.53	19.02	33.17	10.76	5.20	3.09	-	0.23	-
Textile	47.15	5.24	8.03	1.60	1.00	1.00	1.60	0.34	PET: 34.03
Treated Wood	33.58	22.38	25.70	0.91	3.36	3.07	0.91	0.11	PET: 9.86, PVC: 0.12
Mixed Treated wood	29.60	19.73	18.73	2.68	2.89	1.79	2.68	0.09	PET: 21.60 PVC: 0.20
Creosote-treated wood	29.51	19.67	34.02	-	6.15	2.36	-	0.19	ASPH: 8.11
Paper	48.02	12.00	11.61	-	-	-	0.39	0.14	PE: 17.99 PVC: 0.05 CO ₂ i: 9.80

Figure 22 to 28 shows the HHV, N, S and Cl levels of the waste classes consisting of only woody biomass. The waste classes 1131 and 1143 were composed of several components and are therefore shown with their average, maximum and minimum instead of a box plot. It can be seen that the surrogates matched the experimental values well. However, as mentioned, chlorine was not included in the surrogates for most of the waste classes.

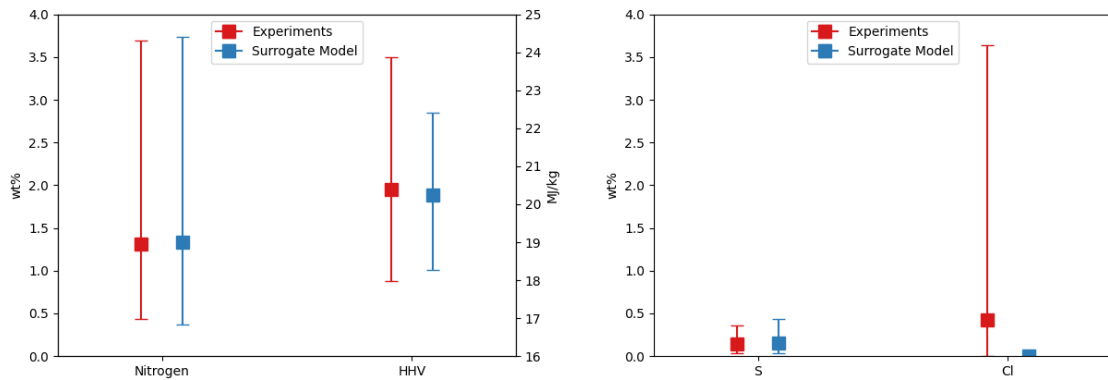


Figure 22: 1131 - Park and garden waste. Plot of the HHV, N, S and Cl contents The square shows the average value, while the whiskers shows the maximum and minimum.

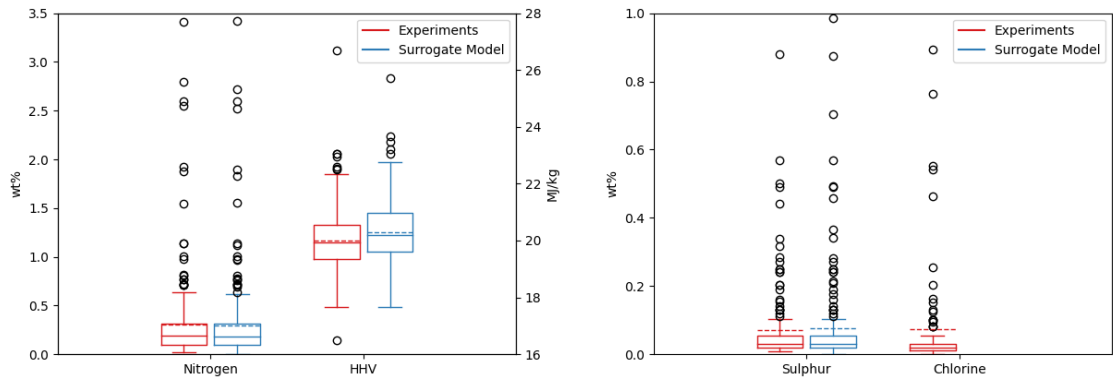


Figure 23: 1141 - Untreated wood. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

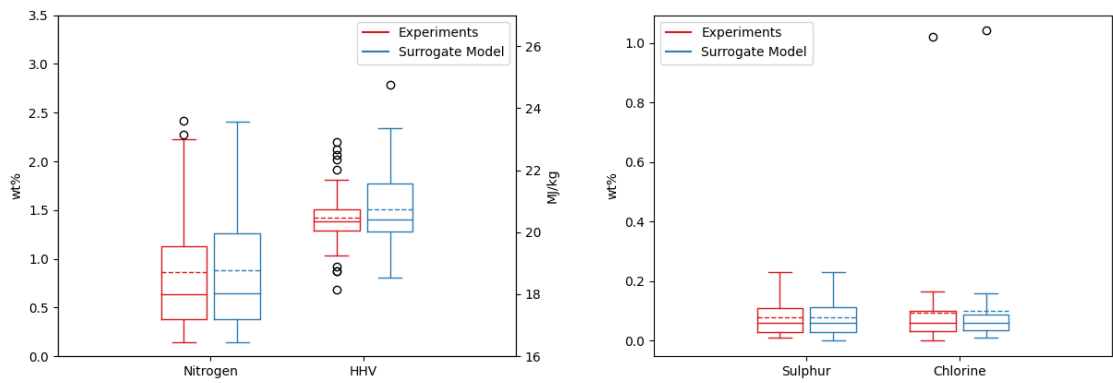


Figure 24: 1142 - Treated wood. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

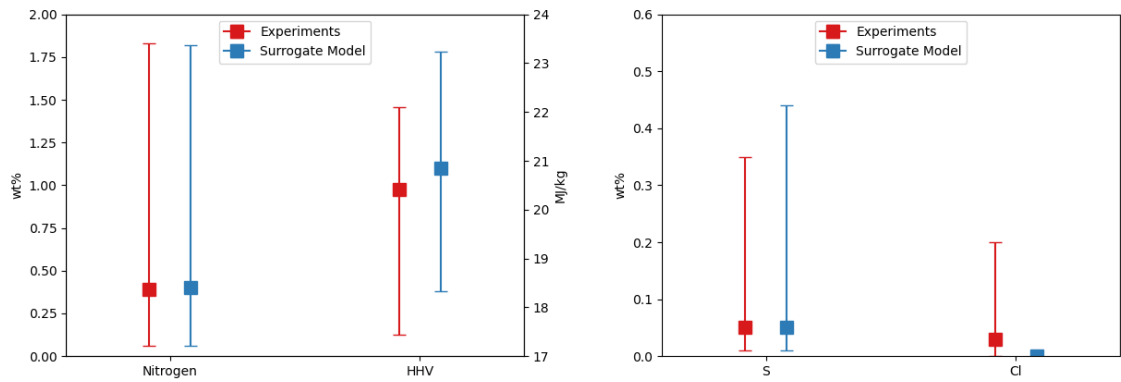


Figure 25: 1143 - Wood chips, shavings, bark. Plot of the HHV, N, S and Cl contents. The square shows the average value, while the whiskers show the maximum and minimum.

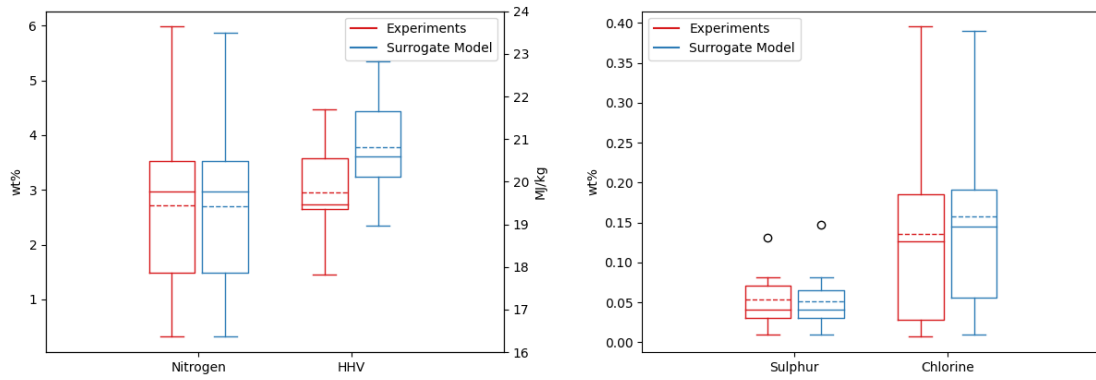


Figure 26: 1149 - Mixed treated wood. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

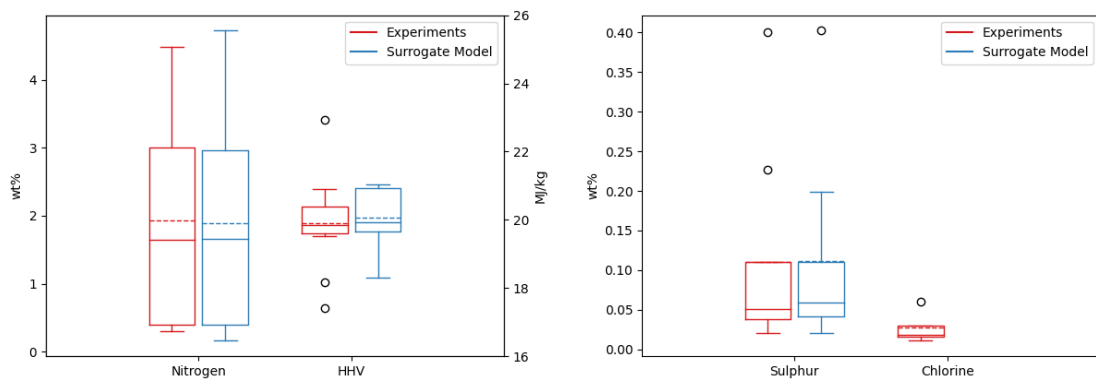


Figure 27: 1912 - Furniture and furnishing. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

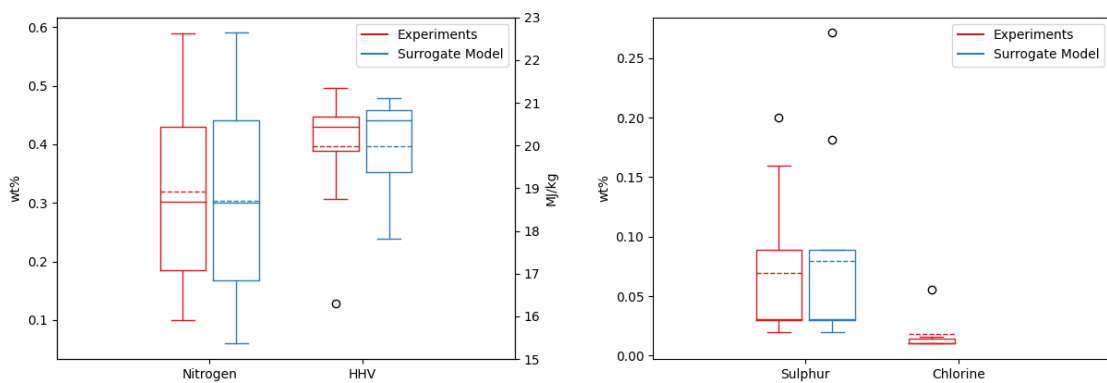


Figure 28: 7098 - CCA-treated wood. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

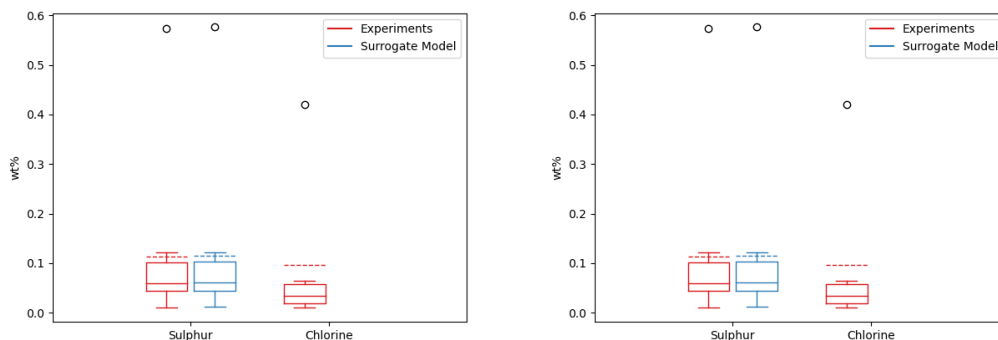


Figure 29: 7154 - Creosote-treated wood. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

4.2 Sludge and other Biomass

The average ultimate analysis and HHV for each component from the surrogates are summarised in Table 21. The table also presents the relative error compared to the experimental data. Table 22 shows the average mass concentration of the surrogate species used in the surrogate formulation.

Table 21: Overview of the elemental composition of the surrogates for sludge and other biomass. The upper row for each component shows the amount of the elements in wt%, and the HHV in MJ/kg. The lower row shows the relative error in % compared to the experimental values

Source	C	H	O	N	S	Cl	HHV
Sewage Sludge	52.926	7.581	29.821	7.327	1.973	0.373	24.405
	0.84	1.64	1.77	0.25	0.20	44.66	6.28
Organic Domestic Waste	51.831	6.265	38.057	2.222	0.726	0.899	21.561
	0.93	0.82	3.52	2.29	4.35	41.36	1.28
Leather	46.097	7.322	31.808	13.079	1.547	0.146	21.386
	0.16	4.32	1.39	12.00	19.00	12.57	11.00
Paper Sludge	47.078	5.732	45.976	0.817	0.252	0.144	18.445
	0.25	2.86	0.22	5.01	1.61	36.28	0.40

Table 22: Composition of surrogate species in wt% for sludge and other biomass

Source	CELL	HCE	LIG	PROT	SUGAR	LIPID	NH ₃ i	CO ₂ i	Sulphur	PVC	PE
Sewage Sludge	7.54	5.02	17.50	27.44	8.29	21.98	4.58	3.74	3.24	0.66	-
Organic Domestic Waste	10.16	6.77	28.96	9.56	14.80	16.20	1.19	9.58	1.19	1.59	-
Leather	-	-	-	84.77	-	9.97	2.46	-	2.55	0.26	-
Paper Sludge	42.57	10.64	17.99	-	-	-	0.99	19.14	0.42	0.25	8.00

Table 19 shows that the surrogates provided accurate results for the components regarding their ultimate analysis. But, it can be seen that the chlorine levels were somewhat wrong for all components. This was because using the surrogate species PVC was the only way to model the chlorine level. However, most of the chlorine content for these waste classes would likely come from organic sources and not PVC plastics. Therefore, adding a new chlorine species for organic materials would make the surrogates for these components more accurate. In addition to the chlorine content, the nitrogen, sulphur and HHV content of leather had a high relative error. This was because the protein in leather is mostly collagen, and the nitrogen level of collagen is higher than the levels of the three protein species used in the model [91]. This indicates that the surrogate formulation for leather needs further improvement, e.g., adding a new protein species.

Table 22 shows the average composition of surrogate species used in the surrogates for each waste component. The surrogate species used for sewage sludge were primarily within limits found by Netzer et al. [12] regarding sewage sludge. Although the amount of sugar and lipid was considerably higher here, but this might be due to different input data.

The surrogates used for the organic domestic waste seem realistic, as this often consists of food and plants. The PVC plastic content is most likely inaccurate since it was added to account for chlorine. In reality, much of the chlorine would come from organic or inorganic sources such as table salt.

The leather component mostly consists of protein and lipid, which is realistic for leather. The inorganic nitrogen, PVC and sulphur species account for additives often used in leather. Using an inorganic chlorine surrogate species instead of PVC could have been more realistic since one can assume that leather does not contain plastics.

The paper sludge was calculated the same way as paper, and the resulting surrogate formulation was quite similar. The big difference was higher lignin and inorganic carbon levels. This might be because lignin is much more durable than cellulose and hemicellulose, and therefore was more lignin left in paper sludge [19].

Figure 30 and 31 show the HHV, N, S and Cl levels of the waste classes consisting of sludge and other biomass. The waste class 1126 was composed of several components and is therefore shown with the average, maximum and minimum instead of a box plot. It can be seen that the surrogates matched the experimental values well.

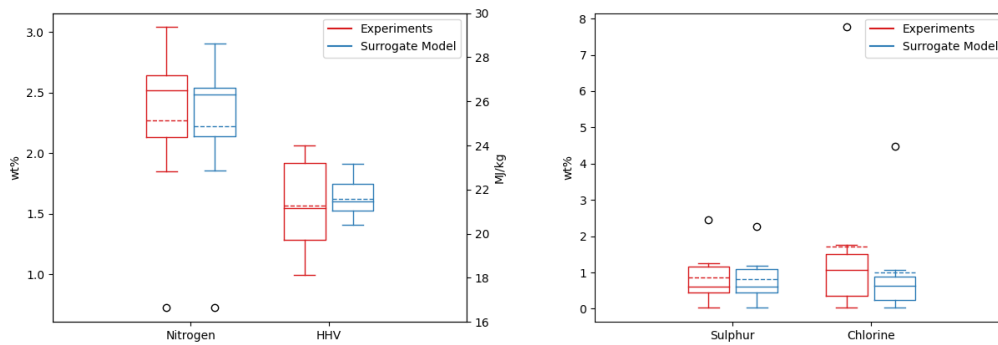


Figure 30: 1111 - Kitchen and food waste from large- and small-scale households. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

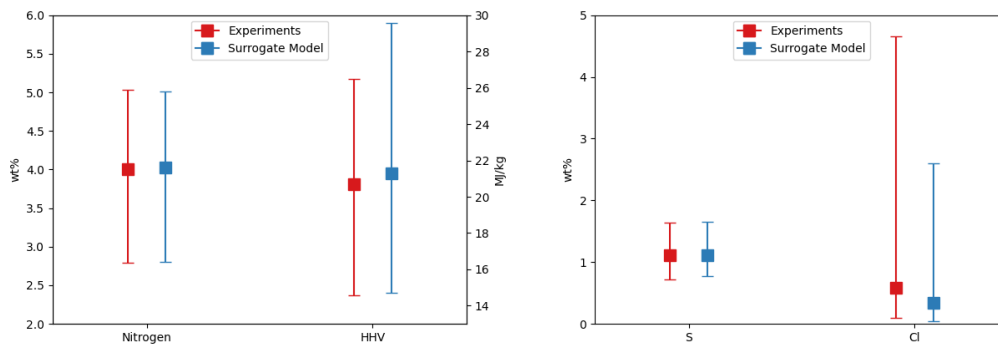


Figure 31: 1126 - Sludge, organic. Plot of the HHV, N, S and Cl contents The square shows the average value, while the whiskers shows the maximum and minimum.

4.3 Mixed Waste

The average ultimate analysis and HHV for each component from the surrogates are summarised in Table 23. The table also presents the relative error compared to the experimental data. Table 24 shows the average mass concentration of the surrogate species used in the surrogate formulation.

Table 23: Overview of the elemental composition of the surrogates for mixed waste. The upper row for each component shows the amount of the elements in wt%, and the HHV in MJ/kg. The lower row shows the relative error in % compared to the experimental values

Source	C	H	O	N	S	Cl	HHV
MSW	55.670	7.494	34.085	2.043	0.541	0.167	24.760
	1.07	0.74	0.90	0.68	1.99	27.71	1.54
Hospital Waste	63.163	7.287	28.490	0.736	0.324	0	27.712
	1.36	14.45	0.06	0.82	9.50	0	5.90
RDF	55.710	7.892	34.534	1.064	0.368	0.433	25.188
	0.77	6.16	0.40	13.68	2.51	16.41	2.19

Table 24: Composition of surrogate species in wt% for mixed waste

Surrogate Species	MSW	Hospital Waste	RDF
CELL	27.11	17.94	30.63
HCE	18.08	11.96	20.42
LIG	5.15	8.80	4.21
SUGAR	6.34	8.66	6.54
LIPID	2.93	2.82	1.69
PROT	6.17	4.39	2.58
NH ₃ i	1.29	0.10	0.74
CO ₂ i	3.88	3.44	3.61
Sulphur	0.89	0.53	0.61
PE	12.51	10.67	17.72
PS	2.45	18.56	1.66
PP	3.13	2.67	4.43
PA	1.48	0.70	0.94
PVC	0.29	0	0.76
PET	5.65	7.02	2.24
NR	2.65	1.73	1.21

Table 23 shows that the ultimate analysis from the surrogates matched the experimental values well, especially for MSW. The exception was the chlorine values, which had a relative error of over 10% for MSW and RDF (while hospital waste had no chlorine in the experimental data). The reason for the inaccurate chlorine values was because the only way to model chlorine was using PVC plastics, while the chlorine in MSW and RDF also comes from organic materials and inorganic chlorine.

The hospital waste overpredicted the H value and underpredicted the S value. However, by looking at the individual data points, it was found that the errors were due to an outlier for both the hydrogen and sulphur values. Since the input for hospital waste was only five data points, one outlier was enough to create a significant error.

For RDF, the relative error of nitrogen was over 10%, and this was because some of the data points had high nitrogen content from the surrogate formulation compared to the experimental values. This might be because the surrogate formulation used too much protein, PA-plastic or inorganic nitrogen for these data points. Nevertheless, aside from these data points, the rest of the values for RDF seemed accurate.

Table 24 shows the average mass concentration of the surrogate species used in the surrogate formulation. The composition for MSW seems plausible since MSW often contains food, plant-

based materials, plastics, rubber and textiles. Hospital waste contained less organic materials compared to MSW. This was expected since hospital waste likely contains more plastic and paper than MSW. The surrogate species used for RDF were similar to those used for MSW. The main difference was that RDF contained lower amounts of protein and lipid, indicating less food waste. This was expected since RDF is often MSW with non-combustible components removed.

Figure 32 to 34 shows the HHV, N, S and Cl levels of the waste classes consisting of mixed waste. It can be seen that the surrogates matches the experimental values quite well. However, it can be seen that the chlorine levels are inaccurate for the reasons explained earlier.

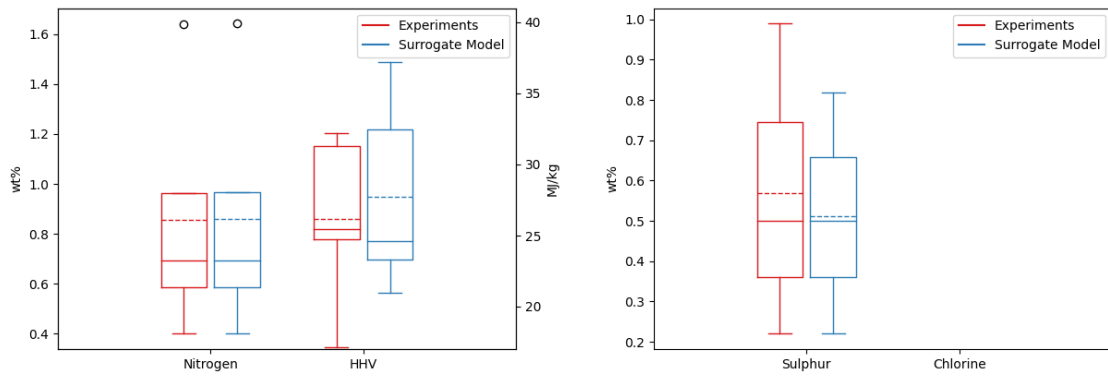


Figure 32: 6004 - Non-infectious waste. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

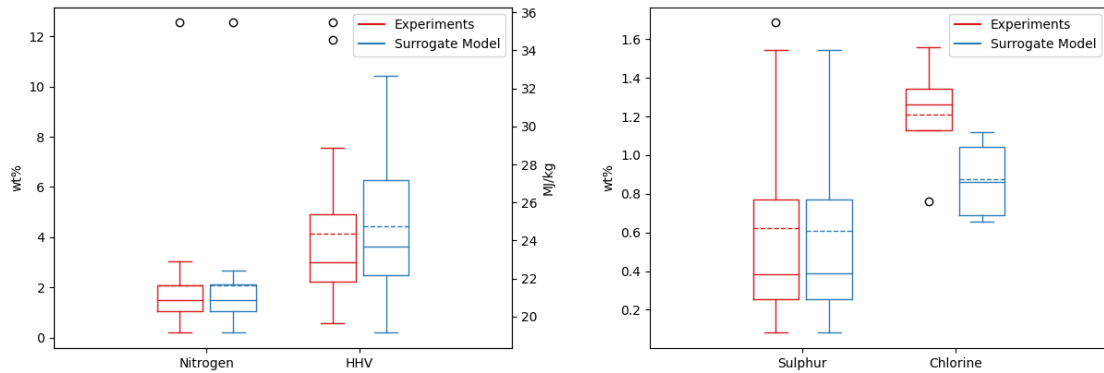


Figure 33: 9911 - Mixed household waste. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

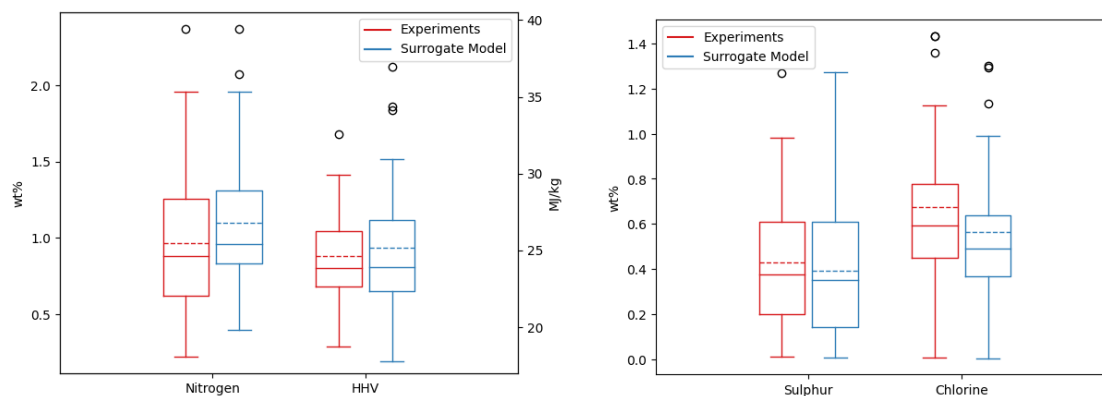


Figure 34: 9913 - Sorted combustible waste. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

4.4 Rubber Waste

The average ultimate analysis and HHV for each component from the surrogates are summarised in Table 25. The table also presents the relative error compared to the experimental data. Table 26 shows the average mass concentration of the surrogate species used in the surrogate formulation.

Table 25: Overview of the elemental composition of the surrogates for rubber waste. The upper row for each component shows the amount of the element in wt%, and the HHV in MJ/kg. The lower row shows the relative error in % compared to the experimental values

Source	C	H	O	N	S	Cl	HHV
Passenger Tyres	84.331	7.824	5.455	0.589	1.773	0.028	38.254
	4.93	5.13	8.93	7.10	8.56	12.5	2.03
Truck Tyres	83.142	7.535	7.021	0.686	1.615	0	37.322
	0.66	2.18	0.62	6.54	0.86	0	1.13
MC/Bike Tyres	80.022	7.108	10.264	0.845	1.761	0	35.408
	3.12	2.66	3.07	4.20	10.38	0	2.23
Mixed Rubber Waste	80.374	7.885	9.466	0.425	1.581	0.271	36.499
	1.04	10.30	0.72	13.97	3.24	15.58	2.76

Table 26: Composition of surrogate species in wt% for rubber waste

Source	CO ₂ i	NH ₃ i	Sulphur	PS	PA	PVC	PET	NR
Passenger Tyres	2.67	0.52	2.92	69.08	1.30	0.05	7.35	16.12
Truck Tyres	3.23	0.57	2.66	68.55	1.74	0	10.88	12.38
MC/Bike Tyres	7.69	0.89	2.90	66.09	0.93	-	10.99	10.52
Mixed Rubber Waste	9.54	0.45	2.60	52.46	0.43	0.48	5.04	29.00

Table 25 shows that the ultimate analysis from the surrogates matched the experimental values well. The relative error was below 10% for most of the elements. Mixed rubber waste had a relative

error above 10% for hydrogen and nitrogen levels, while MC/Bike tyres had a relative error above 10% for sulphur. These errors were due to outliers, which, due to the few data points used, caused significant relative errors. The chlorine levels were inaccurate for passenger tyres and mixed rubber waste due to the low amount of chlorine, which led to minor absolute errors becoming significant relative errors.

Table 26 shows the average composition of the surrogate species used for the surrogates. It can be seen that all waste components consist of high values of PS-plastics. This was due to the decision of using PS-plastic to model synthetic rubber, and the amount used seems realistic, although the amount was overpredicted compared to what is typically found in tyres [58]. Also, the natural rubber content was underpredicted for the components [58]. The combined PET and PA content was between 5 and 13% for all components, which is realistic since the textiles used in tyres often consist of polyester and nylon [58]. The inorganic carbon content was between 2 and 10% for all components and probably accounts for some of the filler used in tyres, which is often carbon black [60]. As for carbon fibre, a surrogate species consisting entirely of carbon could have made the surrogate formulation more accurate. The carbon black might also be the reason for the PS species being overpredicted. Due to the PS species having a high carbon content, it might account for some of the carbon black content. The PVC surrogate species was used for mixed rubber waste and passenger tyres and was added in order to account for the chlorine. It can be seen that the amount of PVC used was minuscule for both waste components.

Figure 35 to 38 shows the HHV, N, S and Cl levels of the waste classes consisting of rubber waste. It can be seen that the surrogates matches the experimental values well.

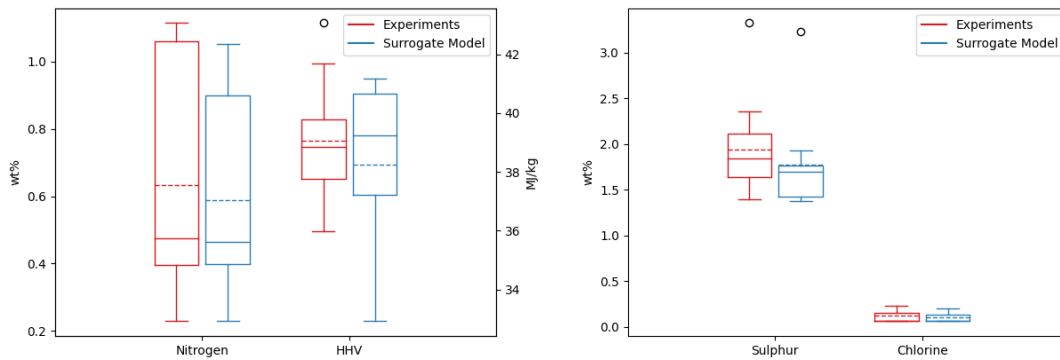


Figure 35: 1811 - Passenger car tyres. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

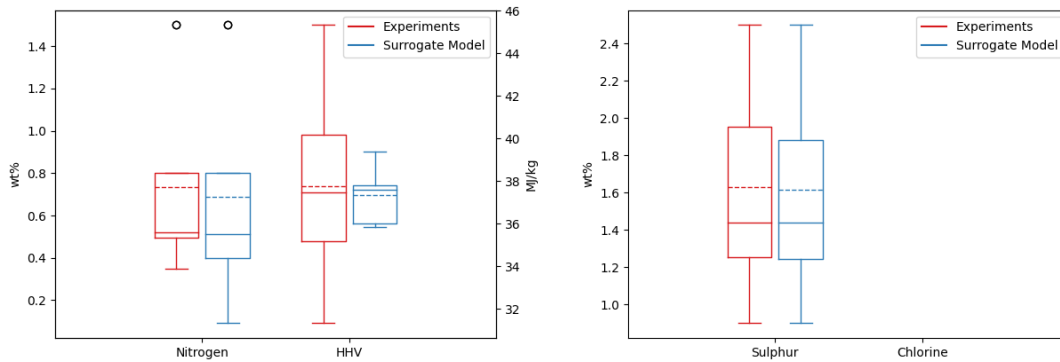


Figure 36: 1812 - Tractor and lorry tyres. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

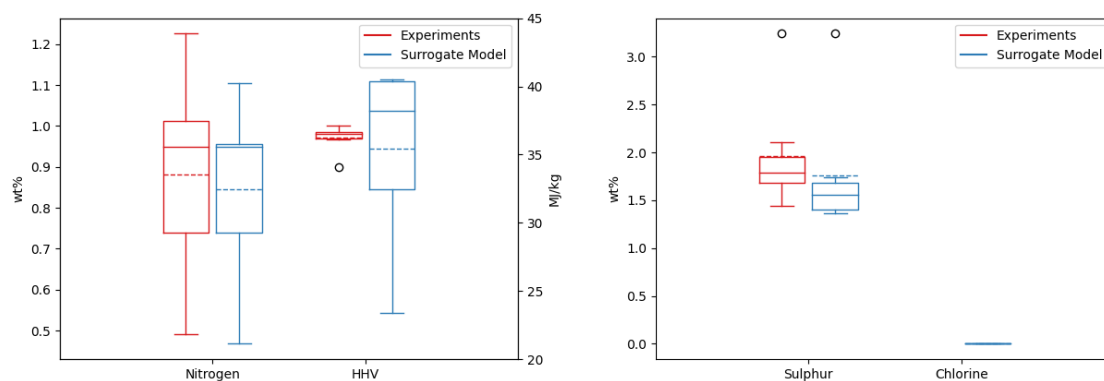


Figure 37: 1814 - Other tyres. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

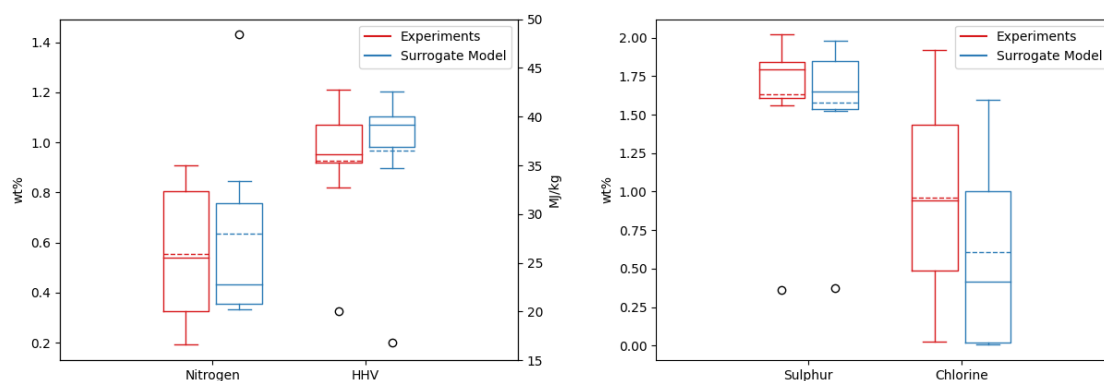


Figure 38: 1899 - Mixed rubber. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

4.5 Plastics

The average ultimate analysis and HHV for each component from the surrogates are summarised in Table 27. The table also presents the relative error compared to the experimental data. Table 28 shows the average mass concentration of the surrogate species used in the surrogate formulation.

The PP, PS, PVC, PE and PET components were described using their respective surrogate species. However, no PET species were available from the surrogate species described in section 2.2, but a new PET species was made in section 3.6. The surrogates should be equal, or almost equal, to the experimental values for all of these components. Still, as seen in Table 27, this was not the case. This was because the experimental values for these components contained some impurities, or the plastics contained additives. Additives are relatively common in plastics, and including these will make them differ from their pure form [92]. This indicates that the surrogates for these components should have been formulated with more surrogate species than just the individual plastic species.

Table 27: Overview of the elemental composition of the surrogates for plastics. The upper row for each component shows the amount of the elements in wt%, and the HHV in MJ/kg. The lower row shows the relative error in % compared to the experimental values

Source	C	H	O	N	S	Cl	HHV
PE	85.628	14.372	0	0	0	0	46.827
	0.26	3.40	100	100	100	0	4.49
PS	92.257	7.743	0	0	0	0	41.33
	0.14	3.16	100	0	100	0	2.74
PP	85.726	14.274	0	0	0	0	46.746
	0.02	0.76	100	0	0	0	1.02
PVC	38.436	4.838	0	0	0	56.726	17.922
	4.09	3.59	100	100	100	6.28	13.02
PET	62.502	4.196	33.302	0	0	0	23.321
	0.93	0.43	2.65	100	100	100	0.82
Carbon-Fibre plastics	82.776	7.904	5.181	2.798	1.34	0	37.767
	3.08	146.46	0.31	41.88	10.90	0	16.07
Glass-fibre plastics	77.849	7.916	11.919	2.107	0.210	0	35.261
	2.48	2.42	5.86	0.05	19.85	0	55.90
Cables	70.615	8.462	19.825	0.218	0.880	0	32.658
	1.90	0.87	8.70	11.79	1856	100	4.85
Synthetic textiles	60.71	4.84	31.72	2.21	0.52	0	23.64
	0.88	4.38	1.55	18.13	101.15	0	5.44

Table 28: Composition of surrogate species in wt% for plastics

Source	PE	PS	PP	PA	PVC	PET	NH _{3i}	CO _{2i}	Sulphur
PE	100	0	0	0	0	0	0	0.0	0
PS	0	100	0	0	0	0	0	0	0
PP	0	0	100	0	0	0	0	0	0
PVC	0	0	0	0	100	0	0	0	0
PET	0	0	0	0	0	100	0	0	0
Carbon fibre	0	71.65	0	21.63	0	4.37	0.15	0.0	2.20
Glass fibre	14.31	52.85	3.58	0.74	0	17.76	2.45	7.97	0.35
Cables	34.47	6.02	8.62	0.16	0.00	41.35	0.24	7.69	1.45
Synthetic textiles	0	0.08	0	11.35	0	84.27	0.98	2.46	0.86

The values for the carbon-fibre plastics had a relative error above 10% for the hydrogen and nitrogen content. This was because carbon fibre contains much carbon, and the surrogates modelled the inorganic carbon using CO₂, which proved unable to model the inorganic carbon since the oxygen level of this surrogate species became too high. Adding a carbon species consisting of pure carbon could have led to better results for the carbon fibre plastics. The other components were reasonably accurate except for the sulphur levels, which had a relative error of over 10% for glass-fibre plastics, synthetic textiles and cables. This might be because the amount of sulphur is low for glass-fibre plastics, so a small absolute error leads to a high relative error. For the cables, one outlier was the reason for the error. Since cables only had five data points, one outlier created a sizeable relative error. This was also the reason for the high relative error of sulphur for synthetic textiles. The chlorine level for cables was also inaccurate, and this was because the input data contained minuscule amounts of chlorine, which was not picked up by the PVC species. The nitrogen content in the surrogate formulation of synthetic textiles was also inaccurate, and this was also due to one outlier.

Table 28 shows the composition of the surrogate species in the surrogates. It can be seen that

the PE, PS, PP, PVC and PET components only contain the surrogate species that it is made of because it was modelled using only the corresponding surrogate species.

It can be seen that carbon fibre plastics primarily consist of the PS surrogate species, which was due to the high carbon content. Since no surrogate species representing pure carbon was used, the model used large amounts of PS plastics since it has a high carbon content. Further validation of the surrogates for carbon fibre plastics, glass fibre plastics and cables was not found.

The synthetic textiles primarily consisted of PA and PET, which was realistic since this is what nylon and polyester are made of [27, 47].

Figure 39 to 42 shows the HHV, N, S and Cl levels of the waste classes consisting of plastics. It can be seen that the surrogates matches the experimental values well. However, it can be seen that the HHV from the surrogates for 1751 and 2431 was overestimated. Also, waste class 7156 was modelled using only the PVC surrogate species, which is why the box plot is only a line for the surrogate. Moreover, as explained earlier, the values from the surrogate formulation did not match the experimental values well for this waste class.

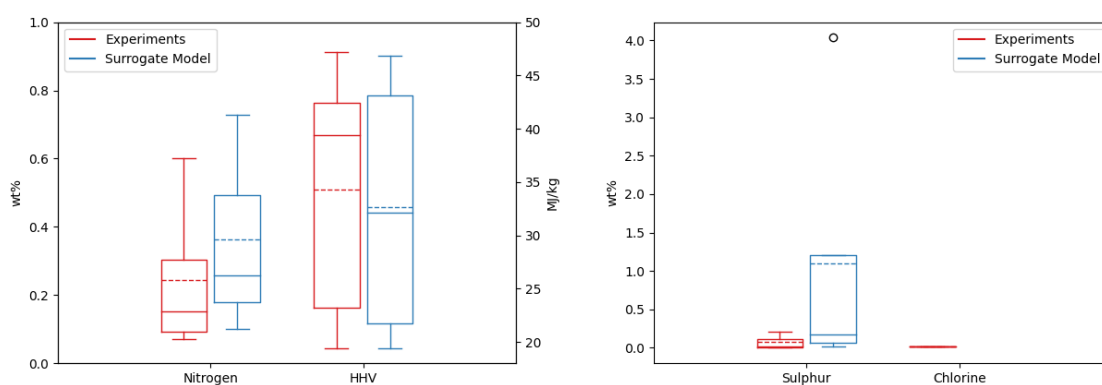


Figure 39: 1504 - Cables. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

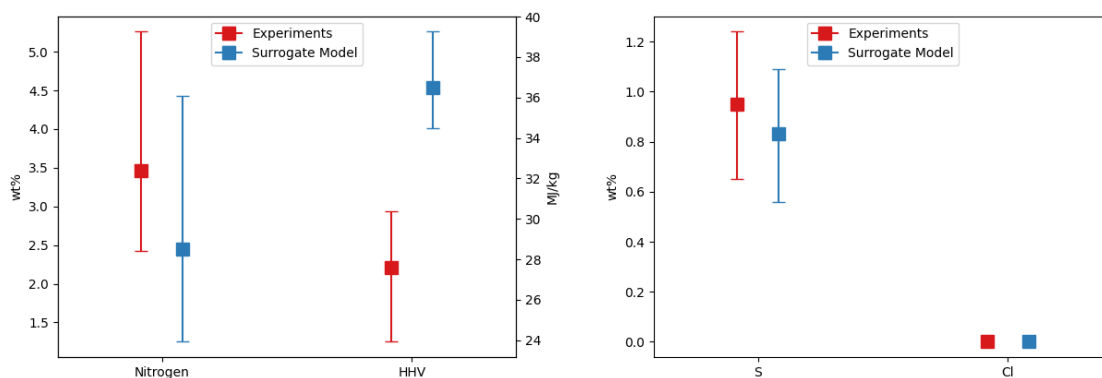


Figure 40: 1751 - Composites. Plot of the HHV, N, S and Cl contents The square shows the average value, while the whiskers shows the maximum and minimum.

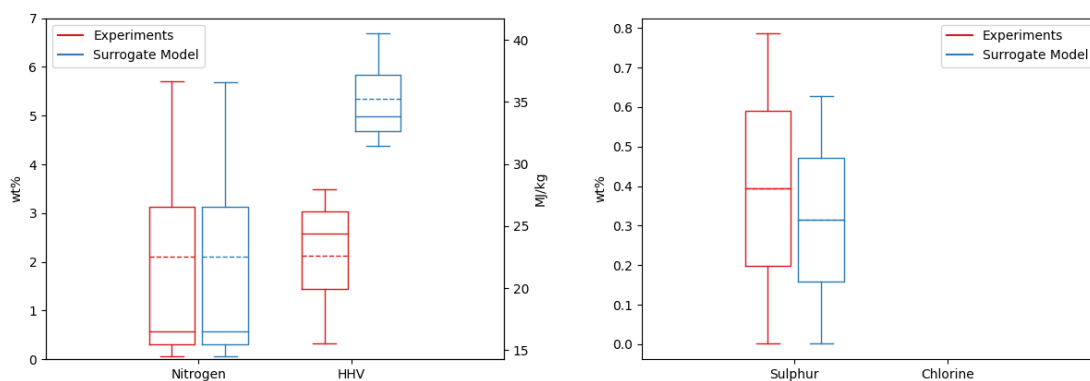


Figure 41: 2431 - Leisure craft. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

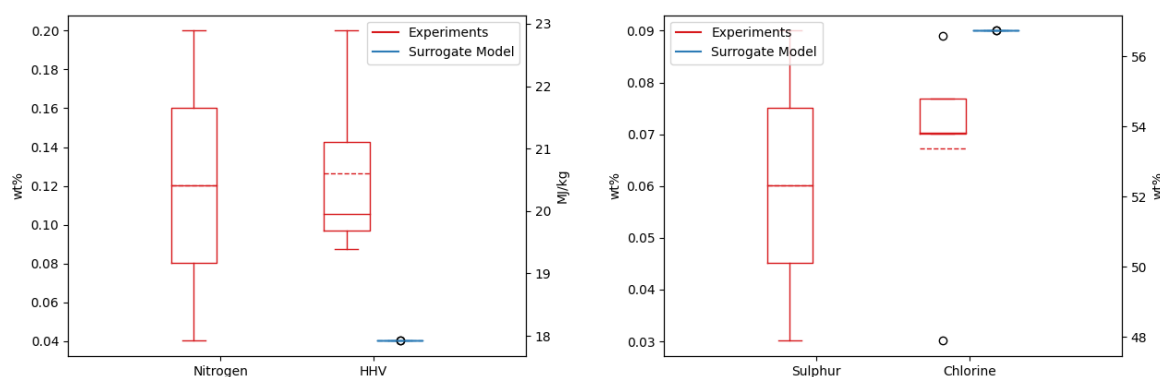


Figure 42: 7156 - Waste containing phthalates. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

4.6 Oil-based Waste

The average ultimate analysis and HHV for each component from the surrogates are summarised in Table 30. The table also presents the relative error compared to the experimental data. Table 29 shows the average mass concentration of the surrogate species used in the surrogate formulation.

Table 30 shows the average ultimate analysis for the surrogates and how it compares to the experimental values. It can be seen that many of the waste components have a high relative error for nitrogen due to the surrogate species asphaltene containing nitrogen. This led to some waste components with a high amount of asphaltene and a low amount of nitrogen to model the nitrogen levels incorrectly. In addition, the sulphur levels were also inaccurate for many of the components. The reason for this was that the hydrocarbon components had relatively high amounts of sulphur but low levels of oxygen. Since the surrogate species used for modelling the sulphur contained about 30% oxygen on a dry-ash-free weight basis, it could not model the amount of sulphur due to the relatively low oxygen levels.

Table 29: Overview of the elemental composition of the surrogates for oil-based waste. The upper row for each component shows the amount of the elements in wt%, and the HHV in MJ/kg. The lower row shows the relative error in % compared to the experimental values

Source	ASPH	PE	PS	Sulphur	CO ₂ i	NH ₃ i
Asphalt	97.03	-	-	2.34	0.62	0
Oil	34.43	51.65	-	3.03	10.48	0.40
Diesel	4.96	94.30	-	0.67	0	0
Distillation residue	82.86	-	-	0	16.73	0.41
Tar	51.62	9.11	-	0.80	33.12	5.36
Activated Carbon	0.91	-	92.48	1.93	3.82	0.85
Oil cuttings	22.84	34.26	-	19.93	22.66	0.30

Table 30: Composition of surrogate species in wt% for oil-based waste

Source	C	H	O	N	S	Cl	HHV
Asphalt	85.159	8.318	2.595	2.503	1.425	0	39.368
	2.31	1.65	29.69	175.96	18.05	0	6.80
Oil	77.416	10.475	9.047	1.221	1.841	0	38.600
	2.26	6.13	7.32	80.89	12.46	0	1.87
Diesel	85.146	13.988	0.315	0.145	0.406	0	46.213
	0.37	0.81	238.71	3.33	20.08	0	1.82
Distillation residue	76.987	7.150	13.389	2.474	0	0	33.880
	2.58	43.57	1.62	3.73	0	0	1.27
Tar	62.014	6.680	25.081	5.737	0.487	0	26.889
	0.49	5.41	0.48	10.92	0.62	0	2.63
Activated Carbon	87.308	7.414	3.380	0.722	1.176	0	38.972
	6.21	84.57	1.57	55.38	15.15	0	6.05
Oil cuttings	57.004	7.182	22.860	0.833	12.119	0	27.205
	7.82	9.93	13.96	16.34	12.17	100	8.22

It can be seen that the hydrogen content for asphalt and distillation residue had a relative error of over 10%. For asphalt, this was because only three data points were used, and one of these significantly overpredicted the hydrogen content. For the distillation residue it might be because the surrogates contained too much asphaltene, which has relatively high hydrogen content. On the other hand, it might be that distillation residue contains significant amounts of inorganic carbon and could have been modelled more correctly if a surrogate species consisting of pure carbon were available. In addition, the distillation residue could have been modelled better if the lipid species had been included in the formulation.

The values for activated carbon were somewhat incorrect, but this was because, as explained in section 3.5.6, a surrogate species for pure carbon was not included in the formulation. Adding a surrogate species for pure carbon could have improved the results for activated carbon. The oxygen level for diesel had a high relative error, probably due to the experimental values of diesel containing minuscule amounts of oxygen (about 0.09 wt%). Since the species asphaltene was used, in addition to the sulphur species, the amount of oxygen became overpredicted in the surrogate formulation

The relative error for oil cuttings was over 10%, which indicates that it was incorrect to model it

the same way as oil. The reason for the deviation was not further analysed, and would be addressed for further work.

Table 29 shows the composition of the surrogate species used for the surrogates. It can be seen that asphalt contains mainly the asphaltene species, with some sulphur and inorganic carbon.

The oil component was modelled using a mix of asphaltene and PE plastic. The PE plastic species were used to model the lighter hydrocarbons. The oil component contained around 10% inorganic carbon, which was used to model the oxygen content correctly. This indicates that including a surrogate species with high oxygen content might have improved the results for oil.

The diesel component was modelled using a mix of asphaltene and PE but with a higher PE content than oil. The surrogate species used seem realistic since diesel mainly contains lighter hydrocarbons [64].

The distillation residue was modelled similarly to asphalt. As explained above, distillation residue might contain significant amounts of inorganic carbon, which might be the reason for the amount of inorganic carbon. On the other hand, significant levels of inorganic carbon in the surrogate formulation might indicate that a surrogate species with considerable oxygen content was missing. Therefore, including the lipid surrogate species could have improved the surrogate formulation for distillation residue.

The tar was modelled similarly to oil but with a higher proportion of asphaltene. The tar surrogate consisted of high amounts of inorganic carbon, which is unrealistic since tar generally consists of hydrocarbons. The considerable amount of inorganic carbon seems to be because the input data had high amounts of oxygen. Since the asphaltene and PE species contain relatively small amounts of oxygen, the model assigned large amounts of inorganic carbon since this is described using CO₂. Therefore, an unrealistic amount of inorganic carbon was used for the tar. The solution to this problem could have been to include lipid as a surrogate species in the surrogate formulation.

Activated carbon was formulated using the PS plastic species. This was because activated carbon consists of pure carbon, and no species for pure carbon was used in this thesis. Therefore, the PS plastic species was used since this contains the largest amount of carbon. However, this led to overpredicted hydrogen values. In order to improve the model for activated carbon, a surrogate species for pure carbon could be added.

The oil cuttings were modelled the same way as oil, and it can be seen that it has the same proportion of PE and asphaltene. However, the amount of sulphur was considerably higher since the sulphur content of the experimental data was significant. In addition, the inorganic carbon level was relatively high. This was probably because of the same reason as for the tar component.

Figure 35 to 38 shows the HHV, N, S and Cl levels of the waste classes consisting of rubber waste. The waste class 7152 was composed of several components and is therefore shown with the average, maximum and minimum instead of a box plot. It can be seen that the surrogates matches the experimental values well. However, the nitrogen level for waste class 7021 was somewhat inaccurate, and this was due to the reasons explained earlier.

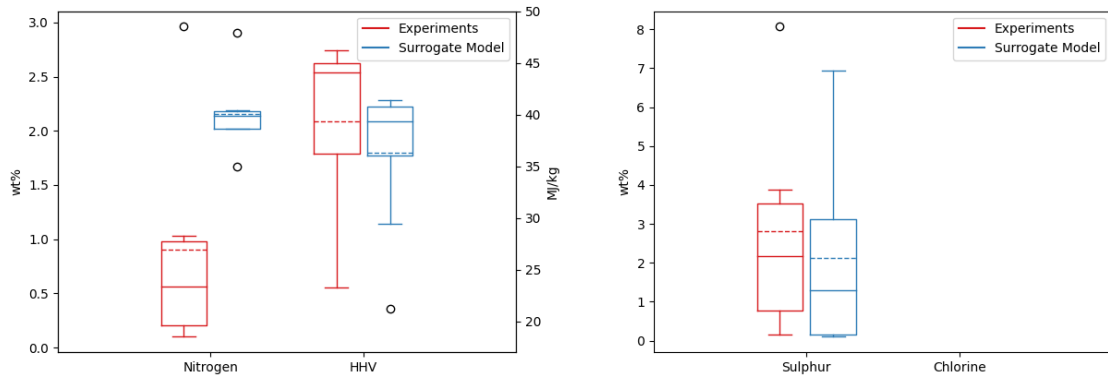


Figure 43: 7021 - Oil and grease. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

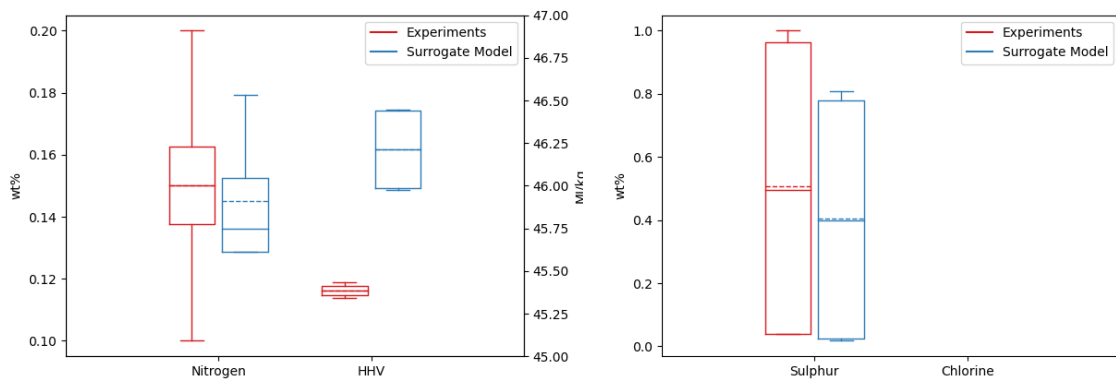


Figure 44: 7142 - Oil-based drilling mud. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

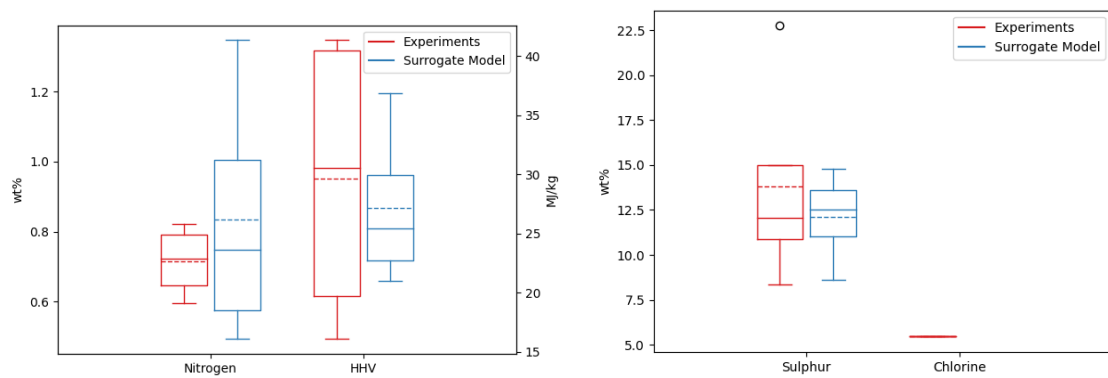


Figure 45: 7143 - Cuttings with oil-based drilling mud. Box plot of the HHV, N, S and Cl contents, the dotted line shows the average.

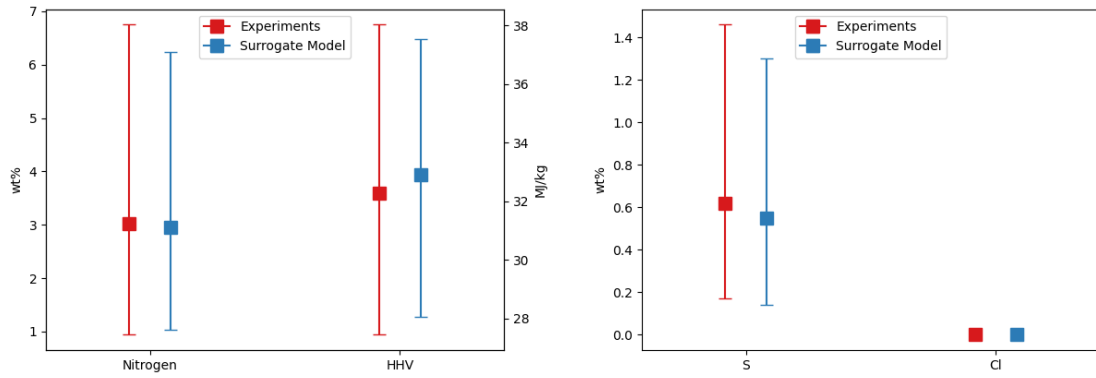


Figure 46: 7152 - Organic waste without halogens. Plot of the HHV, N, S and Cl contents. The square shows the average value, while the whiskers show the maximum and minimum.

4.7 Waste classes with Components from Several Categories

Waste class 1506, 1621, 1911, 7022 and 7024 consists of components from several categories, and are shown in Figure 47 to 51 below. Since all of these waste classes consists of several components they are described using the average, maximum and minimum instead of the box plot. It can be seen that the values from the surrogates matched the experimental values fairly well.

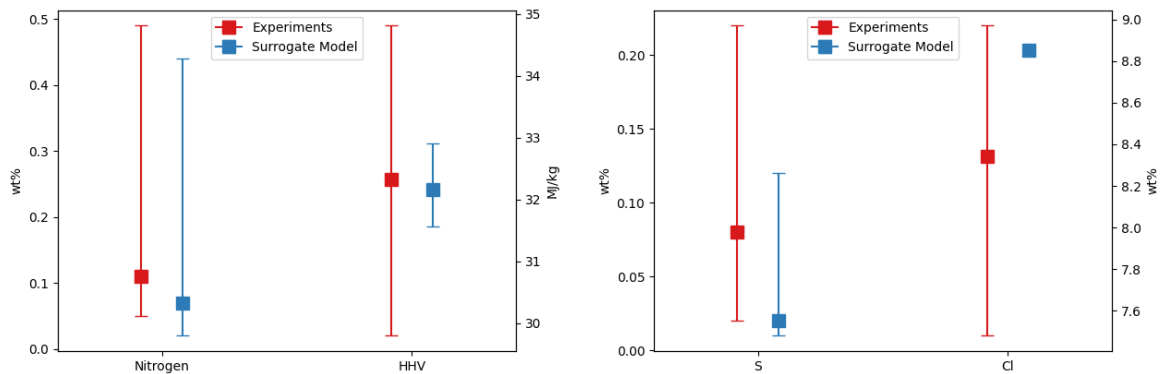


Figure 47: 1506 - Toys, recreational and sports equipment. Plot of the HHV, N, S and Cl contents. The square shows the average value, while the whiskers show the maximum and minimum.

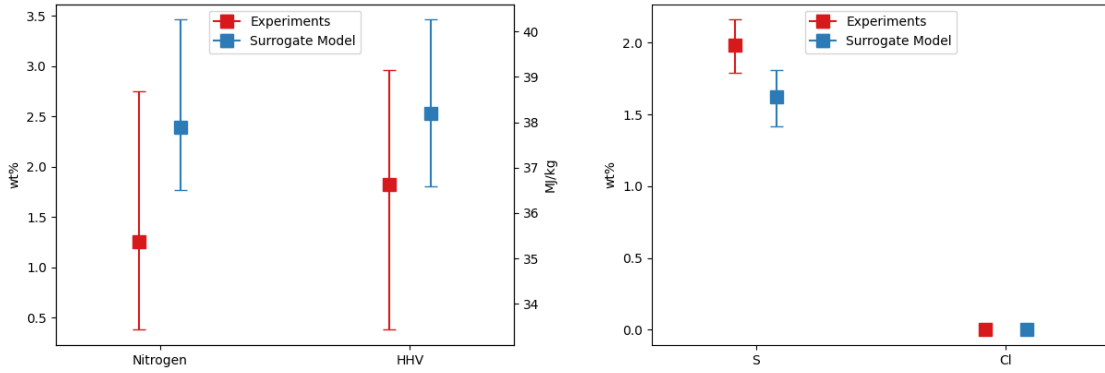


Figure 48: 1621 - Roofing felt/tar paper. Plot of the HHV, N, S and Cl contents The square shows the average value, while the whiskers shows the maximum and minimum.

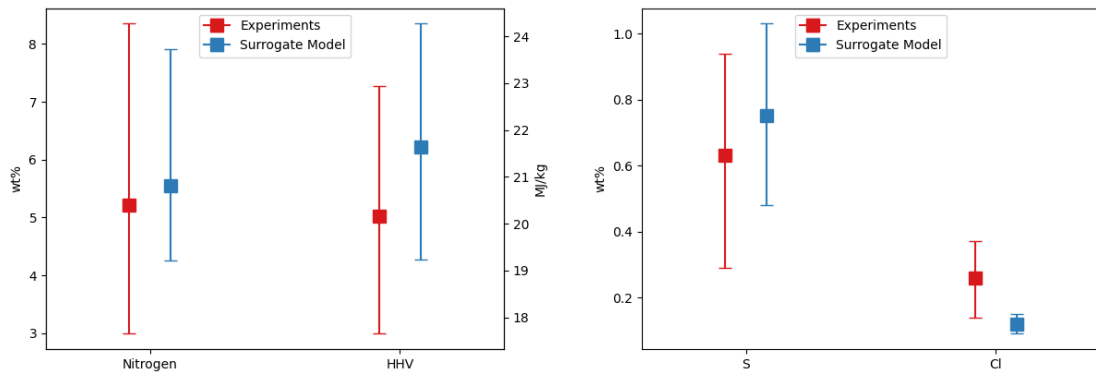


Figure 49: 1911 - Textiles and leather. Plot of the HHV, N, S and Cl contents The square shows the average value, while the whiskers shows the maximum and minimum.

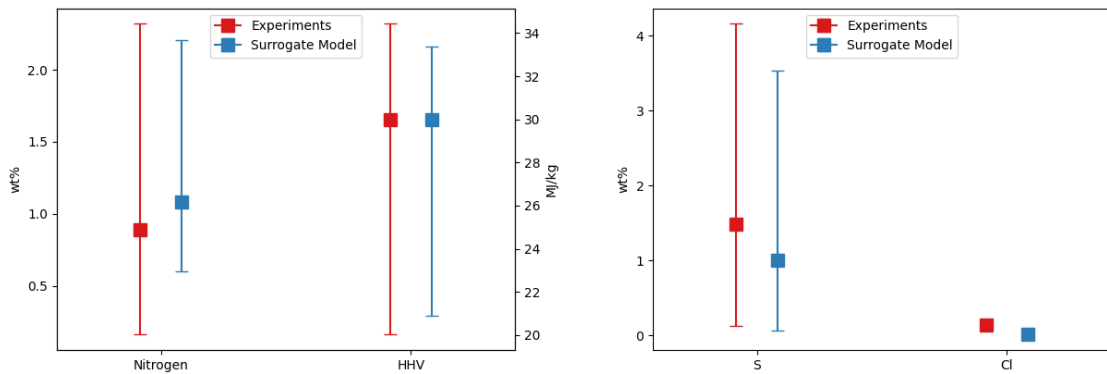


Figure 50: 7022 - Materials contaminated with oil. Plot of the HHV, N, S and Cl contents The square shows the average value, while the whiskers shows the maximum and minimum.

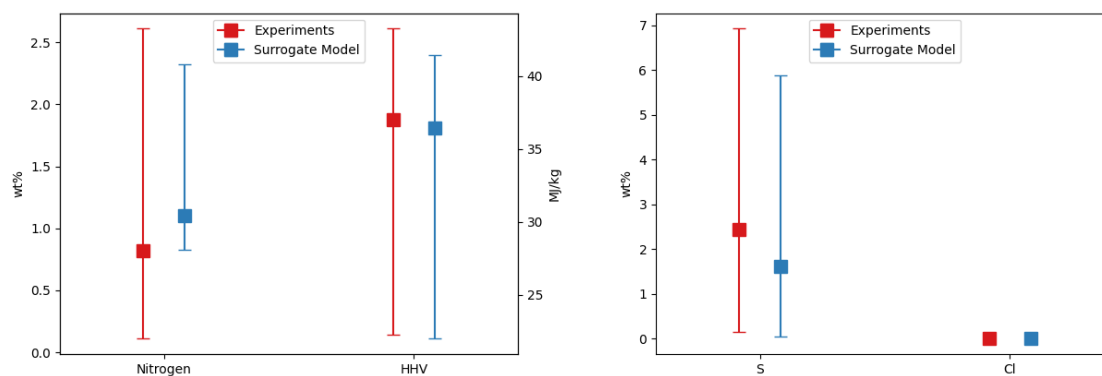


Figure 51: 7024 - Oil filters. Plot of the HHV, N, S and Cl contents. The square shows the average value, while the whiskers show the maximum and minimum.

4.8 Overview of Surrogate Species used for each Waste Class

Table 31 shows the average composition of surrogate species used in the surrogates for each waste class. The composition of surrogate species for each component was discussed earlier and is therefore not discussed here.

4.9 Comparison of the waste classes

Figure 22 to 51 shows the HHV, N, S and Cl content from the surrogates and experimental data. From these some general conclusions can be made about the waste classes.

Waste classes with high content of oil, rubber and plastics have the highest HHV, with most of them having average values between 35 and 40 MJ/kg. Waste classes consisting of organic materials generally had an average HHV of around 20 MJ/kg. The waste classes consisting of mixed waste had an average HHV between 25 and 28 MJ/kg. Mixed waste consists of both rubber and plastics, as well as organic materials, so it was expected that they should have HHV somewhere between these two.

Waste classes consisting of non-woody organic materials such as organic sludge, and textiles and leather had high average nitrogen contents (over 4 wt%). The rest of the waste classes generally had average nitrogen values between 0 and 3 wt%.

Most of the waste classes had average sulphur levels below 1 wt%. The exceptions were waste classes with large proportions of rubber and oil where the average sulphur levels generally were between 1 and 3 wt%. The waste class organic sludge had an average sulphur level of around 1 wt%. One large exception regarding the average sulphur content was cuttings with oil-based drilling mud that had average sulphur levels over 12 wt%.

Almost all waste classes had an average chlorine content under 0.5 wt%, but there were some exceptions. Kitchen and food waste had chlorine contents of around 1 wt%, which was also the case for mixed household waste and sorted combustible waste. Toys, recreational and sports equipment had an average chlorine content of over 8 wt% due to the PVC present in this waste class. Waste containing phthalates had an average chlorine content above 50 wt% due to the fact that this waste class was modelled using only PVC plastic.

Table 31: Composition of surrogate species for all waste classes

Waste Class	CELL	HCE	LIG	PROT	SUGAR	LIPID	NH ₃ i	CO ₂ i	Sulphur	PE	PP	PS	PA	PVC	PET	NR	ASPH
1111 - Kitchen and food waste from large- and small-scale households	10.16	6.77	28.96	9.56	14.80	16.20	1.19	9.58	1.19	-	-	-	-	1.59	-	-	-
1126 - Sludge, organic	25.06	7.83	17.75	13.72	4.15	10.99	2.78	11.44	1.83	4.00	-	-	-	0.46	-	-	-
1131 - Park and garden waste	30.89	20.59	30.57	10.08	6.04	1.60	-	-	0.24	-	-	-	-	-	-	-	-
1141 - Untreated Wood	36.04	24.03	30.11	2.19	4.83	2.70	-	-	0.09	-	-	-	-	-	-	-	-
1142 - Treated Wood	33.58	22.38	25.70	0.91	3.36	3.07	0.91	-	0.11	-	-	-	-	0.12	9.86	-	-
1143 - Wood chips, shavings, bark	30.92	20.62	36.45	2.83	5.91	3.19	-	-	0.07	-	-	-	-	-	-	-	-
1149 - Mixed Treated Wood	29.60	19.73	18.73	2.68	2.89	1.79	2.68	-	0.09	-	-	-	-	0.20	21.60	-	-
1504 - Cables	-	-	-	-	-	-	0.24	7.69	1.45	34.47	8.62	6.02	0.16	0	41.35	-	-
1506 - Toys, recreational and sports equipment	9.25	3.96	4.59	0.24	0.53	0.30	0.04	1.08	0.03	17.58	15.60	15.60	-	15.61	15.60	-	-
1621 - Roofing felt/tar paper	-	-	-	-	-	-	0.70	2.72	1.77	4.09	1.02	15.12	0.21	0	5.08	-	69.28
1751 - Composites	-	-	-	-	-	-	1.30	3.99	1.28	7.16	1.79	62.25	11.19	0	11.07	-	-
1811 - Passenger car tyres	-	-	-	-	-	-	0.52	2.67	2.92	-	-	69.08	1.30	0.05	7.35	16.12	-
1812 - Tractor and lorry tyres	-	-	-	-	-	-	0.57	3.23	2.66	-	-	68.55	1.74	0	10.88	12.38	-
1814 - Other tyres	-	-	-	-	-	-	0.89	7.69	2.90	-	-	66.09	0.93	0	10.99	10.52	-
1899 - Mixed rubber waste	-	-	-	-	-	-	0.45	9.54	2.60	-	-	52.46	0.43	0.48	5.04	29.00	-
1911 - Textiles and leather	15.56	1.73	2.65	28.50	0.33	3.62	1.66	0.81	1.24	0	0	0.03	3.75	0.09	39.04	-	-
1912 - Furniture and furnishing	32.54	21.69	33.32	1.98	6.90	1.43	1.98	-	0.15	-	-	-	-	-	-	-	-
2431 - Leisure craft	-	-	-	-	-	-	2.45	7.97	0.35	14.31	3.58	52.85	0.74	0	17.76	-	-
6004 - Non-infectious waste	17.94	11.96	8.80	4.39	8.66	2.82	0.10	3.44	0.53	10.67	2.67	18.56	0.70	0	7.02	1.73	-
7021 - Waste oil and grease	-	-	-	-	-	-	0.40	10.48	3.03	51.65	-	-	-	-	-	-	34.43
7022 - Materials contaminated with oil	23.76	4.31	4.91	0.40	0.25	0.25	0.70	7.69	1.64	30.32	-	-	-	0.01	8.55	-	17.22
7024 - Oil filters	6.24	1.56	1.51	-	-	-	0.40	10.37	2.65	46.29	-	1.00	0.01	0.02	0.10	0.55	29.30
7098 - CCA-treated wood	40.03	26.69	24.67	2.33	3.82	2.34	-	-	0.11	-	-	-	-	-	-	-	-
7142 - Oil-based drilling mud	-	-	-	-	-	-	0	0	0.67	94.30	-	-	-	-	-	-	4.96
7143 - Cuttings with oil-based drilling mud	-	-	-	-	-	-	0.30	22.66	19.93	34.26	-	-	-	-	-	-	22.84
7152 - Organic waste without halogens	-	-	-	-	-	-	2.18	17.71	0.90	3.01	-	30.52	-	-	-	-	44.68
7154 - Creosote-treated wood	29.51	19.67	34.02	-	6.15	2.36	-	-	0.19	-	-	-	-	-	-	-	8.11
7156 - Waste containing phthalates	-	-	-	-	-	-	-	-	-	-	-	-	-	100	-	-	-
9911 - Mixed household waste	27.11	18.08	5.15	6.17	6.34	2.93	1.29	3.88	0.89	12.51	3.13	2.45	1.48	0.29	5.65	2.65	-
9913 - Sorted combustible waste	30.63	20.42	4.21	2.58	6.54	1.69	0.74	3.61	0.61	17.72	4.43	1.66	0.94	0.76	2.24	1.21	-

5 Conclusion

The goal of this master thesis was to find surrogates for each of the typically incinerated waste classes described in the author's project work. The surrogates were found for all these waste classes, except seven that were not included due to insufficient data material or because they consisted of inorganic materials. The surrogates were calculated using a linear least-square fit between the surrogate species and the experimental dry-ash-free carbon, hydrogen, oxygen, nitrogen, sulphur and chlorine levels for each data point.

The surrogate species used were taken from two models by Netzer et al. regarding municipal solid waste and sewage sludge and extended by new species. Natural rubber was needed to model rubber waste, PET for plastic waste, asphaltene for oil-based waste and an organic chlorine species for the chlorine in organic materials. However, it was found too laborious to create a new surrogate species for organic chlorine due to its occurrence in most waste classes and its unknown accumulation in the char and ashes. The new species were modelled by finding their reaction using previous experiments available in the open literature and testing these reactions using pyrolysis conditions in a stochastic reactor model.

The results showed that most surrogates had a relative error under 10% for the elements and HHV compared to the experimental values. The exceptions were believed to be either due to insufficient data points available, incorrect surrogate formulation or missing surrogate species. As mentioned above, a chlorine species for the organic waste classes were missing, making the surrogates unable to model the chlorine levels for organic waste classes. It was also found that the species used for inorganic carbon, CO_2 , contained too much oxygen to model waste classes containing large amounts of inorganic carbon components (e.g. carbon black, carbon fibre). The oil-based wastes should also have had a surrogate species to model the lighter hydrocarbons since the plastic species PE had to be used for modelling them in this thesis.

Nevertheless, the surrogates for 30 waste classes were found in this master thesis, and most of them proved to have an elemental composition and higher heating value close to the experimental values. Moreover, the composition of surrogate species also seemed realistic for most waste classes. A statistical overview of the waste classes was created based on the surrogates and the experimental values. Therefore, the statistical analysis of the waste classes together with the surrogates can provide more information about the waste classes' fractions (organic versus fossil), elemental composition and heating value. They can also be used as input in numerical models that can calculate the expected emissions and energy output, providing information on how to run waste-to-energy power plants more efficiently. The statistical overview is relevant for stakeholders in waste management and other research, such as life-cycle analysis.

6 Future Work

As mentioned in section 3.6, a surrogate species accounting for the chlorine content in organic materials is needed. Therefore, creating such a surrogate species would probably improve the surrogates for organic waste classes. In addition, as discussed in section 4, including such a species could also improve the surrogates for mixed waste.

As discussed in section 4, the waste classes with high carbon content could have been modelled more accurately if a surrogate species consisting of mostly carbon was used. Future work could therefore be to use such a surrogate species and then examine if this improves the accuracy of the waste classes with high carbon content.

Knowing the composition of surrogate species for the surrogates makes it possible to calculate the amount of carbon from fossil-based sources for each waste class. This information might be beneficial since this tells how much of the CO₂ emissions come from fossil-based sources and, therefore, are not carbon-neutral.

The surrogates could be used as input in a numerical model to model waste incineration emissions and energy output. The results from the numerical model could then be compared to real data from a waste-to-energy power plant. This would provide more information regarding the waste classes and the surrogates accuracy. If the numerical models prove to be accurate, they can then be used to model the emissions and energy output from the waste classes and thus contribute to a more optimal operation of waste-to-energy power plants.

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Appendix

A Representation of the Waste Classes

The following section describing the different waste classes was taken from the author's project work [8]. It was discovered that waste class 1131 - Park and garden waste was written incorrectly, as it was written the same way as 1143 - Wood chips, shavings, bark. Therefore, this was changed below, and the composition of waste class 1131 was made using the distribution of data points, as had been done for many of the other waste classes.

Below is an overview of how the composition and data for each waste class were found. In total 842 different sets of data were found, where 669 were from the Phyllis database and 173 were from previous research. The data found in previous research came from a total of 131 different research articles. All the descriptions for the different waste classes are from the Norwegian Standard NS 9431.E:2011 [7], unless other sources are provided. Several assumptions had to be made since many of the waste classes had little or no previous research regarding their composition and/or properties. However, the assumptions made (except the ones made for simplicity) were sent to Returkraft, and they have confirmed that the guesses are somewhat correct [93]. In reality, the composition of waste might also vary considerably with location and time [94].

1111 - Kitchen and food waste from large- and small-scale households: 15 data sets from the Phyllis database were used to find the averages. The category organic domestic waste from Phyllis was used.

1126 - Sludge, organic: Data from the Phyllis database. It was assumed that the waste class consists of 50% sewage sludge, 41% paper sludge and 9% food sludge. The composition was first assumed based on the composition of data available from the Phyllis database, however, the amount of sewage sludge was decreased after recommendations from Returkraft [93]. It was used 17 data sets to find the averages for sewage sludge, eight for paper sludge and two for food sludge.

1131 - Park and garden waste: Data from the Phyllis database. Using the data available from Phyllis gave a distribution of 56% wood, 34% grass and plants and 10% leaves and needles. The same distribution was assumed for this study. It was used 38 data sets to find the averages for wood, 23 for grass and plants, and seven for leaves and needles.

1141 - Untreated wood: 253 data sets from the Phyllis database were used to find the averages. Using the data for untreated wood available from Phyllis gave a distribution of different wood types as seen in table 32. The same distribution was assumed for this study. For this waste class, the average of all the data sets was used, and not the composition. This was because different wood species are different, but still somewhat similar to each other [95].

Type of wood	Part (%)	Type of wood	Part (%)
Fir/pine/spruce	33	Poplar	5
Oak	9	Pine	4
Beech	7	Willow	4
Eucalyptus	6	others	31

Table 32: Different wood species used for waste class 1141

1142 - Treated wood: 41 data sets from the Phyllis database were used for calculating the averages. This class includes treated wood such as demolition materials, cuttings and wood that has been treated with paint, varnish or chemicals not considered to be hazardous waste.

1143 - Wood chips, shavings, bark: Data from the Phyllis database. Using the data available from Phyllis gave a distribution of 53.5% wood chips, 26.8% bark, 12.7% sawdust and 7% others/mix. The same distribution was assumed for this study. It was used 84 data sets to find the averages for wood chips, 42 for bark, 20 for sawdust and 11 for others/mix.

1149 - Mixed treated wood: Data from the Phyllis database. This waste class consists of

wood that has been manufactured into products such as plywood, particle board, softboard or hardboard. Using the data available from Phyllis gave a distribution of 57% particle board, 29% plywood, 7% hardboard and 7% softboard. The same distribution was assumed for this study. It was used eight data sets to find the averages for particle board, four for plywood, one for softboard and one for hardboard.

1504 - Cables: Five data sets from previous research were used for calculating the averages. The data is for cables where most, or all of the metal is removed.

1506 - Toys, recreational and sports equipment: The Norwegian Standard NS 9431.E:2011 describes this waste class as "Model railways, video games, exercise equipment and other similar equipment" [7]. There was a lack of data for this waste class, both in Phyllis and previous research. In addition, no previous research regarding the composition of this waste class was found. Therefore, it was assumed that it consists of 14% polyvinylchloride (PVC), 14% polypropene (PP), 14% polyethene (PE), 14% polystyrene (PS), 14% polyetylentereftalat(PET), 10% metal (5% aluminium and 5% iron), 10% paper and 10% wood. This was based on assumptions made after briefly looking through one online toy store, and one online sports equipment store, which gave the expression that most of this category consists of plastics [96, 97]. Therefore, it was assumed that this waste class consists of 70% plastic, while the rest is composed of 10% of wood, paper and metals respectively. The plastic was again divided into equal parts of the most common plastics [98]. If more time had been available a more thorough analysis of the distribution and composition of the products should have been done. The average composition and heating value of each material were found by using five data sets for each material. The exception to this is the average value of wood, which is based on the aforementioned waste class 1141. In addition, aluminium and iron are pure metals and therefore have a heating value of zero, and are considered to be ash in the ultimate analysis.

1603 - Slightly polluted soil, inorganic materials etc. and 1604 - Polluted soil, inorganic materials etc.: There was no existing data about these waste classes in the Phyllis database, and the data from previous research often focused exclusively on the trace elements, without including an ultimate analysis or heating values. Nevertheless, two articles regarding the ultimate analysis of soil were found in previous research [99, 100]. Therefore, the data from these articles were used for determining the ultimate analysis for both waste classes, while other previous research was used for determining the trace element composition. In addition, the data regarding the trace elements from previous research had to be assigned to the correct waste class. The Norwegian Standard NS 9431.E:2011 did not provide a way of telling the two waste classes apart, therefore a report from 2009 from the Norwegian Pollution Control Authority was used for telling the waste classes apart [101]. Table 33 show the amount of a substance in mg/kg that is considered hazardous waste according to the report. In this project, the values for the total chromium were used, not the value for chromium(IV). The reason for this is that the data do not specify which type of chromium was measured and therefore the total amount was used. In addition, the report provides equation 30. Inserting the measured trace elements from each data set and the limit values from table 33 into equation 30 gave a number that indicates the state of the soil measured. If this calculated number was higher than one, the soil was considered to be hazardous waste. Therefore, any data set for soil that was over this limit was discarded, since this waste class do not include soil that is considered hazardous waste

To tell the two waste classes apart, figure 52 was used. Here it was assumed that waste class 1603 has values corresponding to class two in figure 52, while class 1604 corresponds to class three to five. Using equation 30 on the values from figure 52, it was found that data with a value between 0.07 and 0.16 are waste class 1603, while data with a value of 0.17 to 1.0 are waste class 1604.

$$\sum = \frac{\text{Measured content of element A}}{\text{Limit hazardous waste element A}} + \dots + \frac{\text{Measured content of element Z}}{\text{Limit hazardous waste element Z}} \quad (30)$$

Substance	Normal values [mg/kg]	Concentration considered hazardous waste [mg/kg]
Arsenic	8	1000
Lead	60	2500
Cadmium	1.5	1000
Mercury	1	1000
Copper	100	25 000
Zinc	200	25 000
Chromium(total)	50	25 000
Chromium(VI)	2	1000
Nickel	60	2500

Table 33: Concentrations of substances considered to be hazardous waste[101]

Tilstandsklasse/ Stoff	1	2	3	4	5
	Meget god	God	Moderat	Dårlig	Svært dårlig
Arsen	< 8	8-20	20-50	50-600	600-1000
Bly	< 60	60 -100	100-300	300-700	700-2500
Kadmium	<1,5	1,5-10	10-15	15-30	30-1000
Kvikksølv	<1	1-2	2-4	4-10	10-1000
Kobber	< 100	100-200	200-1000	1000-8500	8500-25000
Sink	<200	200-500	500-1000	1000-5000	5000-25000
Krom (III)	<50	50-200	200-500	500-2800	2800-25000
Krom (VI)	<2	2-5	5-20	20-80	80-1000
Nikkel	< 60	60- 135	135-200	200-1200	1200-2500
ΣPCB ₇	< 0,01	0,01-0,5	0,5-1	1-5	5-50
DDT	<0,04	0,04-4	4-12	12-30	30-50
ΣPAH ₁₆	<2	2-8	8-50	50-150	150-2500
Benzo(a)pyren	< 0,1	0,1-0,5	0,5- 5	5 -15	15-100
Alifater C8-C10 ¹⁾	< 10	≤10	10-40	40-50	50-20000
Alifater > C10-C12 ¹⁾	< 50	50- 60	60-130	130-300	300-20000
Alifater > C12-C35	< 100	100-300	300-600	600-2000	2000-20000
DEHP	<2,8	2,8-25	25-40	40-60	60-5000
Dioksiner/furaner	<0.00001	0,00001-0,00002	0,00002-0,0001	0,0001-0,00036	0,00036-0,015
Fenol	<0,1	0,1-4	4-40	40-400	400-25000
Benzen ¹⁾	<0,01	0,01-0,015	0,015-0,04	0,04-0,05	0,05-1000
Trikloretan	<0,1	0,1-0,2	0,2-0,6	0,6-0,8	0,8-1000

Figure 52: Categories for polluted soil [101]

1606 - Polluted dredging soil: Data from previous research. As was the case for the aforementioned waste classes 1603 and 1604, there was a lack of data concerning the ultimate analysis and heating value for this waste class. The data from previous research mostly contained information about the trace elements, however, some of them gave the amount of carbon, nitrogen and/or sulphur. These values were included in the report, even though the average value for some of them only consists of the value from one of the sources. None of the data contained information about the heating value, and since the ultimate analysis does not include all the elements, it was also not possible to calculate it.

1614 - Polluted concrete and tiles: Concrete is generally made of water, cement and aggregates, while tiles are generally made of glass, asphalt, plastics or asbestos cement [100, 102]. Here it was assumed that there is no plastic in the tile waste, and therefore it can be assumed that nothing in this waste class is combustible. Therefore, the values of the ultimate analysis and heating values

were assumed to be zero. However, since the waste class consists of only inorganic materials, the ash content was set to 100% [103]. It was further assumed that the trace elements (the pollution) are the same as for waste class 1604. A possible problem with this assumption is that the pollution seen in polluted soil waste might be considerably different than the one seen in polluted concrete and tiles waste.

1621 - Roofing felt/tar paper: No data for this waste class was available in the literature. However, the composition of roofing shingles was found to be approximately 35% limestone filler, 33% granules made from stone, 20% asphalt, 8% fibreglass and 4% backdust made from glass [104]. Since no data for roofing felt could be found, it was assumed that roofing shingles are approximately the same as roofing felt. No data for tar paper was found, but tar paper is generally not used anymore [105]. Since this report focused on the ultimate analysis and heating value for the different waste classes, it was sufficient to find data about the two materials, asphalt and fibreglass, that has heating value and contains elements used in the ultimate analysis. It was used three data sets to calculate the averages for fibreglass and three for asphalt. For this waste class, it was assumed that the rest of the materials are inorganic materials, and therefore classified as ash in the ultimate analysis.

1671 - Cinders, dust, bottom ash and fly ash: Data from the Phyllis database and previous research. It was assumed that this category consists of 57% ash, 21.5% dust and 21.5% cinders. This was based on the composition of data available. It was used eight data sets to calculate the averages for ash, three for dust and three for cinders.

1672 - Blasting sand: Data from previous research. From the data, it was found that blasting sand only contains inorganic materials [106]. Therefore, all the values in the ultimate analysis and heating values were zero, except ash, which was 100%.

1751 - Composites: Data from previous research. It was assumed that composites are glass fibre plastics and carbon fibre plastics. The waste class was therefore assumed to consist of 43% glass fibre, 28.5% carbon fibre and 28.5% mix of composites. This was based on the composition of data available. It was used three data sets to calculate the averages for glass fibre, two for carbon fibre and two for the mix.

1811 - Passenger car tyres: Nine data sets from Phyllis, and four from previous research were used to calculate the average values. Some of the data from Phyllis does not specifically say that the tyre waste is from passenger car tyres, but the proximate and ultimate analysis for these data compared to the data from previous research suggest that this is the case [39]. Therefore, these data sets were included in this waste class.

1812 - Tractor and lorry tyres: Nine data sets from previous research were used for calculating the average values. It was only found data for lorry tyres since there was a lack of data available for tractor tyres. Therefore, it was assumed that tractor and lorry tyres are the same, something that might not be the case in reality.

1813 - Tyres from construction machinery: No data was found for this category. It was therefore assumed that this waste class has the same values as waste class 1812.

1814 - Other tyres: Data from previous research. It was assumed that other tyres consist of bicycle, rickshaw and motorcycle tyres. Therefore, the data consists of 43% motorcycle tyres, 28.5% bike tyres and 28.5% bike/rickshaw tyres. This was based on the composition of data available. It was used three data sets to calculate the averages for motorcycle tyres, two for bike tyres and two for bike/rickshaw tyres.

1899 - Mixed rubber waste Two data sets from Phyllis and five from previous research were used for calculating the average values. It was assumed that this waste class consists of rubber chips and granulates, as well as rubber found in municipal solid waste.

1911 - Textiles and leather Two data points from Phyllis and 12 from previous research. For simplicity it was assumed that this waste class consists of 33% textiles, 33% synthetic textiles and 33% leather. It was used six data sets to calculate the averages for textiles, three for synthetic textiles and five for leather.

1912 - Furniture and furnishing: Four data sets from Phyllis and seven from previous research were used for calculating the average values. The data used for this waste class is mostly wood waste from furniture.

2431 - Leisure craft: No data about the heating value or composition of leisure crafts were found in the literature. Therefore, it was assumed that leisure crafts consist of glass-fibre plastics since most leisure crafts nowadays are made of fibre-reinforced plastic composites [107]. Therefore, four data sets from previous research about glass-fibre plastics were used to calculate the average values. However, this waste class could also contain materials such as wood, metals and other types of plastics, but this was not included in this project.

6004 - Non-infectious waste: Five data sets from previous research were used for calculating the average values. This waste class consists of waste from places such as hospitals, veterinaries, doctor's offices etc. that is not infectious.

7021 - Waste oil and grease: All data from previous research. It was assumed that this waste class consists of 37.5% oil sludge, 25% used motor oil, 12.5% bilge water oil, 12.5% crude oil and 12.5% weathered crude oil. This was based on the composition of data available. It was used three data sets to calculate the average values for oil sludge, two for used motor oil, and one each for the rest of the materials.

7022 - Materials contaminated with oil: All data from previous research. The Norwegian Standard NS 9431.E:2011 describes this waste class as "Input filters. Sludge and other solid oily waste such as bottom sludge from oil separators, soil contaminated by oil, used oil booms and absorbents, separator sludge from ships, bottom sludge from cleaning oil tanks, and oily rags" [7]. For simplicity, it was assumed that the waste class consists of 20% soil, 20% oil sludge, 20% crude oil, 20% cotton cloth and 20% paper. The cotton cloth and paper were added because the waste class includes oily rags and used oil filters made from cardboard [108]. For this waste class, it was assumed that the soil has a heating value of zero. The same data as for waste class 7021 were used to find the averages for oil sludge, while one data set each was used for crude oil and cotton cloth. The average values for the paper were the same as for waste class 1506.

7024 - Oil filters: No data specifically about oil filters was found in previous research. However, an article from 1997 provides data about the composition and amount of oil found in used oil filters [109]. There it was found that used oil filters contain 45-60 wt% of used motor oil and that a new oil filter is made up of 80.6% steel, 16.9% paper and 2.5% rubber. By combining these two numbers, and assuming that the used oil content is 52.5%, it was found that used oil filters consist of 52.5% used motor oil, 38.3% steel, 8% paper and 1.2% rubber. The average values for used motor oil were the same as the ones for waste class 7021, the composition of steel was assumed to be 72.4% iron, 18.3% chromium, 8.0% Nickel, 0.8% Manganese and 0.3% Silicon [110], and its heating value is zero. The data for paper was the same as the ones found for waste class 1506, while the data for rubber was the same as for waste class 1899.

7051 - Paints, glues and varnishes: There was little data about the ultimate analysis and heating values of this waste class in previous research. However, one report about the composition of paint waste in Denmark was found and was used for this waste class [111]. The article provided data about the composition of paint waste in two Danish cities, and the trace elements, moisture content and higher heating value for each component. There was no data for the ultimate analysis of the components and these were therefore not included. The exception was the value of sulphur, which was included in the report. Taking the average waste composition from the cities gave that the waste class consists of 69% water-based paint, 7% solvent-based paint, 6% water-based wood impregnation, 10% solvent-based wood impregnation, 1% water-based lacquer, 2% solvent-based lacquer and 5% glue.

7098 - CCA-treated wood: Six data sets from Phyllis and five from previous research were used for calculating the average values. This waste class consists of wood that has been treated with chromate copper arsenate (CCA) [112].

7142 - Oil-based drilling mud: No data specifically about oil-based drilling mud was found. Oil-based drilling mud is a drilling mud with oil, often diesel oil, as the fluid matrix [113]. A 2015

article gave the composition of oil-based drilling mud as shown in table 34 [114]. Neglecting the emulsifiers, filter loss agent and NaOH while applying a density of diesel oil of 834 kg/m^3 [64] and water of 997 kg/m^3 [115], gave a wt% distribution of 59% diesel oil, 31% water, 7% bentonite and 3% barite. Bentonite and barite are minerals and were therefore classified as ash in the ultimate analysis, while the water content was classified as moisture. Therefore, the ultimate analysis and heating values were found using existing research on diesel oil [116].

Mud component		Mud component	
Oil (mL)	245	Water(mL)	105
Primary emulsifier(mL)	6	Bentonite(g)	25
Secondary emulsifier(mL)	4	NaOH(g)	0.25
Barite(g)	10		

Table 34: Composition of oil-based drilling mud [114]

7143 - Cuttings with oil-based drilling mud: Seven data sets from previous research were used to calculate the average values. This waste class consists of cuttings containing oil-based drilling mud [108].

7145 - Cuttings with water-based drilling mud that contain dangerous substances: No data specifically about this waste class was found. However, water-based drilling mud either contains no or negligible amounts of the elements used in the ultimate analysis and therefore it has a heating value of zero [117, 118, 119, 120]. As for waste classes 1614 and 1672, this waste class consists of 100% ash in the ultimate analysis.

7152 - Organic waste without halogens: The Norwegian Standard NS 9431.E:2011 describes this waste class as "Solid, liquid and gaseous waste such as distillation residues, tar waste, reaction residues, by-products and used absorbents" [7]. No data specifically about this waste class was found. Therefore it was for simplicity assumed that it consists of 33% tar, 33% distillation residues and 33% activated carbon. Four data sets were used to calculate the average values for activated carbon, three for tar and four for the distillation residue.

7154 - Creosote-treated wood: Six data sets from the Phyllis database and five from previous research was used for calculating the average values. This waste class mostly consists of railroad ties and telephone poles, since these have often been treated with creosote [48].

7156 - Waste containing phthalates: The description in the Norwegian Standard NS 9431.E:2011 states that phthalates are primarily used as softening agents in plastics, particularly PVC plastics. Therefore, it was assumed that this waste class consists of PVC plastics. Five data sets from previous research were used for finding the average values.

9911 and 9912 - Mixed household waste and mixed commercial waste: Nine data sets from Phyllis and 13 from previous research was used for calculating the average values. Waste classes 9911 and 9912 consist of mixed waste from households and commercial activities, also called municipal solid waste [121]. It was assumed that waste class 9912, which is mixed waste from public and private enterprises, is the same as waste class 9911. In addition, the data used contains two data sets regarding the mixed waste from shops. In reality, there might be some difference between these two waste classes since households and enterprises produce a somewhat different composition of waste [122]

9913 - Sorted combustible waste: 30 data sets from the Phyllis database were used for calculating the average values. For this waste class, the data regarding Reuse-Derived-Fuel (RDF) from Phyllis has been used. RDF is a fuel made of combustible waste, such as paper, plastics (not PVC) and cardboard [57]. Since RDF consists of the combustible parts of waste, it is fair to assume that sorted combustible waste and RDF have the same properties.

B LOGEResearch setup

Figure 53, 54 and 55 shows the ignition used settings and gas composition used in LOGEResearch.

```
GasPhase
  Molefraction
    AR = 1.0
  END
  TEMPERATURE = 300.
  PRESSURE = 1.013e5
  MASSFLOW = 1.0422e-3
END
SurfacePhase = "SURFMECH1"
PHASEFRACTION
PE = 0.99
ASH = 0.01
  END
  TEMPERATURE = 300.0
END_OF_FILE
```

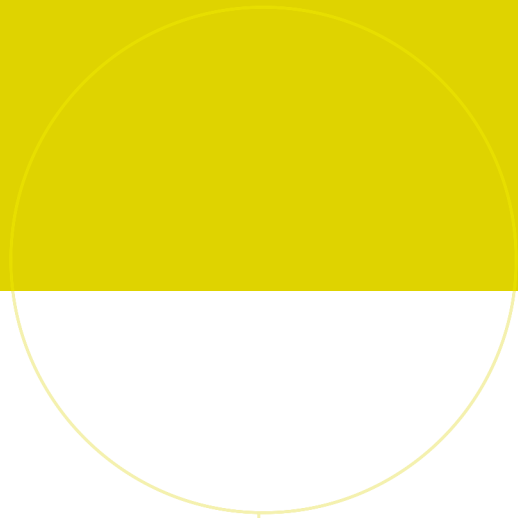
Figure 53: Gas composition setup

```
ID = "22d6e"
REACTOR_TYPE = 54
ASCII_CHEMISTRY
END_OF_LIST
PDF_DATA
  LOCKED_STOCHASTIC = 1
  MIXING_MODEL = 3
  TAU = 1.0
  BETA = 1.0
  STOCON = 15.0
  NBR_OF_PARTICLES = 3
  MAX_NBR_OF_PARTICLES = 6
END_OF_LIST
OUTPUT_OPTIONS
  MASSFRACTION
  N_STEPSBETWEENOUTPUT = 50
END_OF_LIST
SOLVER_SETTINGS
  DT_MIN = 1.0e-11
  DT_MAX = 0.01
  BDF_MAXORDER = 5
  INSTATIONARY
  ABSOLUTE_TOLERANCE = 1.0e-12
  RELATIVE_TOLERANCE = 1.0e-8
  N_ITERATION_STEPSMAX = 10
  N_DAMP_STEPSMAX = 3
  N_MODIFIED_STEPSMAX = 20
  N_TIMESTEPS_MAX = 1000000000
  ADVANCE = 1.0
  LIMIT_RATES
  FNM_FLAG = 2
  SOLVERVERSION = 2
END OF LIST
```

Figure 54: Ignition user settings 1

```
ID = "22d6e"  
REACTOR_TYPE = 54  
ASCII_CHEMISTRY  
END_OF_LIST  
PDF_DATA  
  LOCKED_STOCHASTIC = 1  
  MIXING_MODEL = 3  
  TAU = 1.0  
  BETA = 1.0  
  STOCON = 15.0  
  NBR_OF_PARTICLES = 3  
  MAX_NBR_OF_PARTICLES = 6  
END_OF_LIST  
OUTPUT_OPTIONS  
  MASSFRACTION  
  N_STEPSBETWEENOUTPUT = 50  
END_OF_LIST  
SOLVER_SETTINGS  
  DT_MIN = 1.0e-11  
  DT_MAX = 0.01  
  BDF_MAXORDER = 5  
  INSTATIONARY  
  ABSOLUTE_TOLERANCE = 1.0e-12  
  RELATIVE_TOLERANCE = 1.0e-8  
  N_ITERATION_STEPSMAX = 10  
  N_DAMP_STEPSMAX = 3  
  N_MODIFIED_STEPSMAX = 20  
  N_TIMESTEPS_MAX = 1000000000  
  ADVANCE = 1.0  
  LIMIT_RATES  
  FNM_FLAG = 2  
» SOLVERVERSION = 2  
END OF LIST
```

Figure 55: Ignition user settings 2



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