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Production of Dissolving Pulp from Oat Husks

Process Design with Techno-Economic and Environmental Assessment in a Life Cycle Perspective

Master's thesis in Innovative and Sustainable Chemical Engineering

AMANDA ULEFORS

DEPARTMENT OF CHEMISTRY AND CHEMICAL ENGINEERING

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Supervisor: Maria Hernández Leal and Tomas Rydberg, IVL
Examiner: Diana Bernin, Chemistry and Chemical Engineering

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Department of Chemistry and Chemical Engineering
Division of Chemical Engineering Chalmers University of Technology
SE-412 96 Gothenburg
Telephone +46 31 772 1000

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Abstract

To face the environmental concerns arising in the world, a green industrial revolution is required. Presently, the textile industry highly contributes to these environmental concerns and, thus, needs to play its part in the revolution. Textile producing processes needs to be adapted to reduce their environmental impact and alternative raw material needs to be identified to contribute to a green, circular economy. Agricultural residues might be one part of the solution. In this thesis, the production of dissolving pulp for the textile industry, from the agricultural residue oat husks, is evaluated. By a techno-economic and environmental assessment, in a life cycle perspective, the purpose of this thesis is to assess the possibilities of implementing oat husks as a raw material for the production of dissolving pulp in industrial scale. The technical assessment has been performed by simulating a scale-up of a lab process in Aspen Plus, based on provided lab data and conducted mass and energy balances. The results from the simulation have been implemented as a life cycle inventory in the environmental assessment, which has been carried out as a prospective life cycle assessment in the software GaBi. Furthermore, the expected capital and operating costs for the potential plant as well as the break-even price of the pulp have been determined. Uncertainties in the results are seen mainly due to the chemical recovery not being part of the simulation of the process. The results from the techno-economic assessment as well as the environmental assessment indicate potential for oat husks as a favourable alternative raw material in the textile industry.

Keywords: textile, dissolving, pulp, circular, green, oat, husks, residue, scale-up.

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Amanda Ulefors, Gothenburg, May 2022

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Introduction

1.1 Background

The global textile industry is facing a variety of challenges, which are accelerating as the demand of clothing and textiles is increasing. The textile industry is a major contributor to the release of greenhouse gas emissions and toxins to the environment as well as large amounts of waste. In 2015, the textile industry was estimated to have caused 1 715 million tons of CO_2 emissions and generated 92 million tons of waste, globally [4]. With an increasing demand, renewable and biodegradable resources are a necessity to reduce the textile industries impacts on the environment.

Polyester, which is made out of fossil fuels and is non-biodegradable, is today the major textile fibre on the market. In 2020, polyester accounted for 52% of the global fibre production where 14.7% was made of recycled polyester [5]. Cotton is a renewable alternative and stands for approximately a third of the produced fibres globally, however, its water footprint is huge [5]. In 2015, 79 billion cubic metres of water was used in the textile industry alone [4]. In order to reduce negative impacts on the environment, man-made cellulosic fibres have been developed. In 2020, man-made cellulosic fibres accounted for approximately 6% of the global fibre production volume. The major man-made cellulosic fiber is viscose, which is made from wood [5]. The increase in demand for textiles is putting pressure on the textile industry to find alternative renewable raw materials, which does not compete with food nor lead to degradation of lands.

TreeToTextile is a Swedish company who considers cellulose to be a part of the solution. The company produces textile fibres from a cellulose rich dissolving pulp, often derived from wood, without the use of harmful toxins [6]. Dissolving pulp can be created in a kraft pulping process, where sodium hydroxide and sodium sulphide are used as active chemicals. When performing a pulping process similar to the kraft pulping process, with sodium hydroxide as the only active chemical, it is called soda cooking [7]. Following the production of dissolving pulp, TreeToTexile's process produces textile staple fibres in an alkaline wet-spinning process [8]. However, there is an interest in the textile industry in finding alternative cellulose rich feedstocks to decrease the demand of wood and increase the resource efficiency of the process. By using residues as raw material, a circular economy would be enabled. The residual streams, which are expected to be of interest have their origin in agriculture, whereof oat husks is one of them.

By using oat husks to create dissolving pulp, an economic value could possibly be added to the residual. The vision is, hence, to create a circular and bio-based textile industry, where TreeToTextile takes the lead and closes the loop.

1.2 Aim

The master thesis aims to perform an upscaling of a lab process, where dissolving pulp is created from oat husks with the intent to be used for production of textile fibres. The purpose is to, through an techno-economic analysis in a life cycle perspective, provide an understanding of how the process would perform in industrial scale - technically, economically and environmentally.

1.3 Scope

There is a time limitation of approximately 20 weeks for this master thesis. Due to this time limitation, the master thesis will only investigate the potential for producing dissolving pulp from oat husks and will not assess other alternative raw materials. Other agriculture residuals will, however, be investigated in the post doc project *Circular cellulose to textile fiber production*, which this master thesis is a part of. This thesis will focus on the potential of using oat husks as a raw material for dissolving pulp. Thereby, alternative uses for oat husks and how these might be affected by extracting oat husks for dissolving pulp purposes, will not be covered.

The techno-economic and environmental assessment in this thesis will be based on results from lab trials. The lab trials, where different raw materials and process conditions are investigated, will however not be included in this thesis.

The different steps of the up-scaled process will be designed using the software Aspen. The input and output streams, which will be given by the process modelling in Aspen, will be analysed in a prospective life cycle assessment, using the software GaBi.

1.3.1 Specification of issue under investigation

This thesis will be a part of a post doc project, which is a cooperation between IVL, Chalmers University of Technology, Stora Enso and TreeToTextile. The project aims at enabling industrial production of textile fiber from cellulose rich residuals, for use in TreeToTextile's process. This in order to enable a circular bioeconomy.

The main issue, which this thesis will investigate, is the performance and impact of the process for production of dissolving pulp from oat husk, which later will be compared with dissolving pulp from wood. The data and information about process conditions needed for the up-scaling of the process, and then later in the LCA, will be based on results from a laboratory study conducted at Chalmers University of

Technology. This master thesis will consider technical and economic aspects by performing an up-scaling in Aspen, and environmental aspects in a life cycle assessment (LCA). Thereby, the project will be divided into two main parts.

1. **Techno-economic assessment**
From data given from lab trials, mass and heat balances will be calculated and a flow diagram will be drawn. The process will be modelled in an industrial scale in Aspen. Process integration will be performed for chemical recovery and heat recovery. Finally, an economic assessment will be carried out.

2. **Environmental assessment**
The data given from the up-scaled process will be used to determine the environmental impacts of the process in a prospective LCA, using GaBi.

2

Theory

2.1 Lignocellulosic biomass

The cell wall of lignocellulosic biomass consists of carbohydrates, lignin and a small portion of extractives. The carbohydrates includes cellulose and different hemicelluloses. The dominating group of hemicelluloses, as well as the ratio of cellulose, hemicelluloses, lignin and extractives, greatly depends on the type of biomass. Commonly, however, is cellulose the dominating component of a plant's cell wall [9].

Cellulose is a linear, non-branched, polysaccharide with $1 \rightarrow 4\beta$-glycosidic bonds connecting the glucose units. In the cell wall, cellulose forms fibrils, which forms so called matrices between each other. In these matrices, hemicelluloses are found and together, the cellulose and most hemicelluloses provide support to the cell wall [10]. Hemicelluloses are often present in a lesser degree than cellulose, even though they often constitute up to a third of the cell wall. Most hemicelluloses are branched linear polysaccharides, in contrast to the non-branched cellulose polymer. The two main groups of hemicelluloses are xylans and glucomannans [9]. Lignin differs both in structure and function from the carbohydrates. Instead of being a linear polysaccharide, its structure is very complex and still not fully known [11]. Lignin is found together with hemicelluloses in the cell wall, where it fixates cellulose and hemicelluloses in a matrix [9].

2.2 Dissolving pulp

Dissolving pulp can be derived from different raw materials, such as wood, cotton and bamboo. Wood is presently the most used raw material, whereof both softwoods and hardwood can be used [12]. In a following process, textiles can be produced from the dissolving pulp as it possesses some special characteristics. Firstly, dissolving pulp distinguishes from other types of pulp mainly in means of alpha-cellulose content. The alpha-cellulose content of dissolving pulp is very high, higher than 90% in general and even higher for pulps produced in a prehydrolysis kraft process. Consequently, the hemicelluloses and lignin content of dissolving pulp must be kept very low [12].

An additional important factor for the characteristics of dissolving pulp is its intrinsic viscosity, which is a measure of the molecular weight of the polymers. A desirable intrinsic viscosity for dissolving pulp is approximately 400-600 mL/g [13]

[12]. The intrinsic viscosity affects the properties of both the pulp and the textile, both in regard to physical strength and how it will react to different textile finishing treatments. Furthermore, for textile purposes, a dissolving pulp benefits from a uniform molecular weight distribution and a high reactivity [12]. The reactivity of the pulp is dependent on the morphology of the cellulose as it affects the chemical accessibility [13].

2.2.1 Oat husks as raw material for dissolving pulp

Oat husks comprise approximately 30% of the oat weight and differs from wood not only in form and size but also in composition [14] [15]. The cell wall of oat husks consists to approximately one third of hemicelluloses, xylan being the most dominating one, and slightly less of cellulose and lignin [15]. Oat husks, thereby, have a lower content of cellulose than wood, which usually have a cellulose content above 40% [13].

Today, oat husks are mainly used as raw material for energy production and as animal feed [14].

2.3 The prehydrolysis kraft process

The kraft process was discovered in 1879 by Dahl and is today the most common process to produce chemical pulp from wood. The kraft process is an alkaline process, producing strong pulps [7].

2.3.1 Pretreatment

When a pulp is to be produced from wood, mechanical pretreatment of the wood is required. The mechanical pretreatment involves important steps, such as debarking and chipping [13]. Debarking is essential to decrease the amount of chemicals needed in both the cooking and bleaching steps and to improve chemical recovery [16]. The bark can be removed by a couple of different technologies, whereof rotating drums and rotary debarkers are most common [13]. Thereafter, the wood needs to be cut into smaller, uniformed chips to improve the accessibility of chemicals, to reduce the required cooking time and improve the pulp quality [17]. In pulp mills, disc chippers are commonly used to cut wood logs into smaller chips. Prior to the alkaline pulping process, the wood chips are screened, by mechanical or wind screening, to sort the chips based size and dimension. The chips are, thereafter, stored before being used for pulping [13].

The alkaline process alone, is not capable of producing a dissolving pulp, due to the hemicelluloses not being sufficiently removed merely from kraft pulping. To improve the hydrolysis and dissolution of hemicelluloses, the hemicelluloses are solubilized in an additional chemical pretreatment step, called prehydrolysis [12]. In the prehydrolysis, hemicelluloses are hydrolysed in water, in an acidic solution or in concentrated acid at a temperature of 160-180°C, 120-140°C or 40°C, respectively.

The dilute acid commonly consists of 0.3-0.5% H_2SO_4 and the concentrated acid of 20-30% HCl. Commercially, the prehydrolysis is carried out in the digester, prior to pulping [13].

2.3.2 Pulping

Kraft pulping consists of a couple of different steps, where the wood chips are delignified. Pulping is also known as cooking [7]. The wood chips are treated with white liquor, an aqueous solution of the active chemicals sodium hydroxide and sodium sulfide, at a temperature of 140°C to 170°C [13]. In Finland 1997, a softwood kraft, recovering most chemicals within the mill itself, was estimated to have a fresh requirement of sodium hydroxide of 20-25 kg per ton of air-dried pulp (Adt) [18]. Along with lignin extraction, cooking causes a certain degree of carbohydrate losses. Cooking hence, results in a cellulose rich pulp and a black liquor containing the dissolved biomass components as well as chemicals [13]. The cooking can be performed batch wise or continuously, in batch or continuous digesters [7].

The stationary vertical cylinder is the most common conventional batch digester; however, this sort of batch cooking system is not as widely used today as it once were. Presently, batch cooking is mainly applied in a sub-wise manner, in which a high-quality pulp is produced. Sub-wise batch cooking reduces the requirements of active chemicals and energy through integration between the batches [7]. In general, at least four digesters of 150-400 m^3 are used. The tall and slim vertical flow digesters are the dominating continous digester in industry. In contrast to batch cooking, continuous cooking is usually performed in one or two vessels, and the process occurs continuously [7].

Due to the complex structure of fiber cell wall of wood chips, the delignification can easily become uneven, in such a way that the chemicals do not reach all fibres to the same degree for the same amount of time. An uneven delignification would result in some fibres being overcooked while others would not react at all. To ensure a more homogeneous delignification of the wood chips, impregnation of the wood chips is essential [13]. By steaming the wood chips, air hindering chemical penetration will be removed. Steaming can be performed through thermal expansion, increasing the vapour pressure or by creating a partial pressure gradient. The efficiency of steaming will increase with increased pressure, temperature and treatment time, since the harsher conditions improves the penetration of white liquor into the wood chips [7]. Through diffusion, the chemicals are transferred into the chips and the dissolved compounds are exiting the chips [13].

2.3.3 Washing

Washing of the pulp is commonly performed after cooking and after bleaching [13]. The aim is to extract the dissolved compounds, especially lignin due to its darkening effect on the pulp, as well as the added chemicals from the pulp [19]. Washing can be performed in many different types of washers and is usually performed in a series of 3 to 4 washers [20]. Regardless of which washing equipment is used, they all provide three important functions - dewatering, displacement and thickening. Common washing equipment are rotary drum washes and belt washers, where the pulp is washed in a rotating drum or while distributed on a wire [13]. As washing usually is carried out counter-currently, the cleanest water will wash the cleanest pulp and the most contaminated wash water will wash the most contaminated pulp [21]. Commercially, washing requires approximately 2 to 3 tonnes of washing water per ton of pulp [20]. The washing performed after cooking is finalized by a screening step to separate undesired particles and fiber bundles from the pulp, before entering the bleaching sequence [18].

The content of the waste water is dependent on both raw material and bleaching sequence, both in regard to carbohydrates and chemicals [21]. The wastewater is treated in two main steps. In the first, primary treatment, solids are extracted from the waste water through screening, sedimentation or neutralisation. Following the primary treatment, the secondary, biological treatment aims at reducing the organic matter content. The biological treatment is usually performed by an activated sludge method or in aerated ponds [21].

2.3.4 Bleaching

After cooking, the lignin content of the pulp is still too high and the pulp is still slightly brown. By adjusting the conditions or the cooking time, harsher conditions would be created, and the pulp would become whiter [13]. However, this would also lead to increased hydrolysis of the carbohydrates and, thus, a reduction in pulp quality [9]. Therefore, to reduce the lignin content without reducing the pulp quality, bleaching is performed. The purpose of bleaching is to make the pulp whiter by reducing the amount of residual lignin [18]. Bleaching can be performed by different means. Historically, chlorine bleaching has been a common bleaching method. However, due to the formation of chlorinated organic compounds, chlorine bleaching was replaced by elemental chlorine-free bleaching processes [22]. Today, bleaching is primarily performed by the use of oxygen, hydrogen peroxide and ozone processes. An unbleached kraft pulp generally have an ISO of 20%, which is a measure of its brightness based on the ISO standard, while dissolving pulp requires 95% ISO [13].

Commonly, bleaching is performed in different stages. These stages are often very similar; however, the reactors differ slightly. In general, up-flow reactors are used for the majority of the stages in a modern plant. Furthermore, a pressurized reactor is required for bleaching at temperatures at or above 100°C. At lower temperatures, an atmospheric reactor is used instead. Finally, the size of the reactor or towers depends on the required bleaching time [7].

In a kraft pulping process, oxygen delignification is a common way of treating the pulp prior to bleaching. The purpose of oxygen delignification is to improve the brightness of the pulp, make the pulp cleaner and hence, decreasing the amount of required bleaching chemicals in the following bleaching sequence [18]. Oxygen delignification is performed at approximately 100°C, in alkaline conditions, usually in two reactors [7]. Oxygen delignified softwood pulp can through hydrogen peroxide bleaching be bleached to a high degree. The high brightness is achieve by the addition a chelating agent, such as DTPA or EDTA, to reduce the content of metal ions, which otherwise would hinder the hydrogen peroxide bleaching [7]. The hydrogen peroxide stage can be used as a delignification or as a bleaching stage, depending on its placement in the bleaching sequence. When hydrogen peroxide is used as a bleaching stage, alkaline conditions and a temperature of 80-110°C, are applied and the stage is usually carried out for one to three hours in an atmospheric environment [7]. The bleaching sequence greatly depends on the wanted quality of the pulp. When a dissolving pulp is desired, a common strategy is to begin the bleaching sequence with oxygen delignification, which is followed by a chlorination stage, an extraction stage, an additional chlorination stage and finally, the bleaching sequence is finalized with a hypochlorite stage [19].

Finally, pulp is often pressed to a dry content of 50% and is thereafter dried to a dry content of 90%. To dry a pulp from 50% to 90%, the water needs to evaporate, which requires an evaporation energy of approximately 2263 kJ per kg of water [23].

2.3.5 Chemical recovery

After cooking, the pulp and the black liquor exits the digester and the black liquor is removed from the pulp through counter current washing. The black liquor is treated in evaporation towers, to concentrate the black liquor by evaporating the water [13]. The extracted condensed water can then be reused in the washing plants [7]. The chemical concentration is then re-increased by the introduction of make-up sodium sulphate [13]. Thereafter, the organic compounds in the strong black liquor are combusted in a recovery boiler, whereof heat is recovered from the generation of hot flue gases [7]. The energy recovered in the recovery boiler usually covers the energy demand of the kraft mill and potential surplus energy can be sold. In general, a recovery boiler recovers 3.5 kg of steam per kg of black liquor dry solids [24].

The smelt recovered from the recovery boiler, which mostly contains sodium carbonate and sodium sulphide, is dissolved in a water solution to obtain green liquor [13]. The green liquor will, besides sodium carbonate and sodium sulphide, also contain some additional salts as well as green liquor sludge. The green liquor sludge is removed in a clarification step before further processing [7]. The green liquor is processed in the white liquor preparation plant, where calcium oxide is added to obtained slaked lime. In the causticizing reaction, sodium hydroxide is formed and thus, white liquor is generated and can be sent to the digesters [13]. The causticizing reaction have an efficiency of approximately 75-85% [20]. Solid lime mud is also obtained in the causticizing reaction and is separated from the sodium hydroxide through filtration or thickening [13]. The lime mud is burned in a lime kiln, whereof the calcium carbonate is calcined and calcium oxide, which can be recycled and used to obtain slaked lime, is formed [7]. In addition, sulphuric acid being derived from the black liquor can be used to form tall oil soap [25].

2.4 Upscaling of a lab pulping process

Scaling up a process from lab scale to industrial scale is a complex process where one needs to consider some different aspects [26]. First off, it is important to make sure the desired pH remains when increasing the dimensions of the flows, since this will have a great impact on the efficiency of the different treatments. Furthermore, in a larger scale, the time for the different process steps will have to be increased due to the larger volumes [13]. Additionally, pressures are often increased in industry, which causes harsher conditions. Under harsher conditions e.g., the chemical inputs can be reduced and still provide the same efficiency [13].

In lab scale, certain types of equipment can be used to perform the process. In industrial scale, however, larger, more complex process units are required, which may affect the different process steps [26]. As an example, in industrial scale, pre-hydrolysis and cooking is usually performed in the same process unit, while in lab scale, this is easier to perform as two separate steps. An additional washing step is also often performed between the two steps, which does not occur in industry.

The washing steps in lab scale does not have to consider not wasting too much water to the same extent as in industrial scale. In industry, the water is often recirculated to decrease the demand even further [26]. As an example, in lab scale, you might use four litres of water to wash 200 g of pulp. If the same ratio of washing water and pulp was to be applied in industry, this would lead to an enormous and unreasonably high demand of wash water.

In a lab trial, most units runs on electricity. In industry, the electricity demand can in general be reduced, since heat can be recovered within the process and used to run most of the process units [13].

2.5 Mass and energy balances

The conservation of mass within a system involves the material entering and exiting the system, as well as the material consumed, produced and accumulated within the system. When no material is consumed or produced, this conservation can be defined as follows

$$m_{in} - m_{out} = acc. \tag{2.1}$$

where m_{in} represent the mass input, m_{out} the mass output and *acc.* the accumulation [27]. When no mass is accumulated, the equation can be rewritten as

$$m_{in} = m_{out} \tag{2.2}$$

which describes how the amount of mass entering a system is equal to the amount of mass exiting the system.

Energy conservation can be described similarly to mass conservation. The first law of thermodynamics, the law of energy conservation, hence include the input, output, consumption, generation and accumulation of energy. Furthermore, energy can exist in different forms and the energy balance is, thus, quite complex [27].

In a closed, steady-state system, where terms describing kinetic and potential energy, as well as work, can be neglected, a heat balance can be described as

$$Q = Q_{reac} + Q_{heat} \tag{2.3}$$

where Q is the total heat load, Q_{reac} is the heat generated by a reaction within the system and Q_{heat} is the heat requirement of the system [27]. When no reaction occurs in the system, the heat load of the system can simply be calculated as

$$Q_{tot} = \sum_{i=0}^{n} Q_{heat} = \sum_{i=0}^{n} m_n \cdot c_{p,n} \cdot \Delta T \tag{2.4}$$

where m_n is the mass of component n, c_p, n is the heat capacity of component n and ΔT is the desired temperature increased [27].

2.5.1 Heat transfer and heat exchangers

Heat transfer through a surface can be expressed as seen in the following in equation

$$Q = U \cdot A \cdot \Delta T_m \tag{2.5}$$

where U is the overall heat transfer coefficient, A the heat transfer area and $\Delta \mathrm{T}_m$ the mean temperature difference [27].

The mean temperature difference is defined as

$$\Delta T_m = \frac{(T_{H,in} - T_{C,out}) - (T_{H,out} - T_{C,in})}{ln\frac{(T_{H,in} - T_{C,out})}{(T_{H,out} - T_{C,in})}} \tag{2.6}$$

where $T_{H,in}$ is the temperature of the hot stream heating the cold stream, $T_{C,out}$ the temperature which the cold stream is heated to, $T_{H,out}$ the temperature of the hot stream after heating the cold stream and $T_{C,in}$ the temperature of the cold stream to be heated [27].

To determine the capital cost, C_c of a heat exchanger, the following equation can be implemented

$$C_c = a + b \cdot A^n \tag{2.7}$$

where a and b are cost constants and n an exponent to represent the type of equipment. For a u-tube shell and tube heat exchanger, a is 10 000, b is 88 and n equals 1 [27].

3

Techno-economic assessment

3.1 Previously conducted lab trial

In lab scale, oat husks have been treated to create dissolving pulp at Chalmers University of Technology. The lab trials have been performed prior to and alongside this master thesis and are, hence, not directly a part of this thesis. The lab trails have rather acted as a source of data and information, which have set a foundation for the work performed in this thesis.

3.1.1 Lab process

The lab trial which seemed most promising and of which this thesis is based on, was performed as a prehydrolysis soda pulping process and a flow chart of this is visualised in Figure A.1. No mechanical pretreatment of the oat husks was needed, since these already are much smaller than wood chips. Instead, the oat husks were directly exposed to prehydrolysis, where they were treated in an acid solution of 0.1 wt% hydrochloric acid for 60 minutes at a temperature of 160°C. Following the prehydrolysis, the pretreated mass was washed and the dissolved components, being mostly hydrolysed hemicelluloses but also ash and lignin, and hydrochloric acid were separated from the mass by vacuum filtration.

After washing and filtration, the mass was cooked for 120 min at 170°C in a 4 wt% sodium hydroxide solution. The cooked pulp was then washed and filtered to remove the black liquor. To ensure separation of the cellulose fibres, defibration was performed. In order to reduce the lignin content even further, the pulp was bleached in two stages for 120 min each, in a 5 wt% hydrogen peroxide solution with 0.01 M sodium hydroxide at 80°C. As a final step, the pulp was washed and filtered and a bright, low lignin content, dissolving pulp was received.

Upon request, a similar lab trial was performed, where the prehydrolysis was performed with 0.0137 M sulphuric acid instead of hydrochloric acid. In this trial, all conditions and following steps remained as in the previously described trial.

Analyses of the pulp content in the lab have been provided as data for the following tasks in this master thesis, see Table A.1 for provided data of the composition of oat husks.

3.2 Method

The techno-economic assessment has been performed based on provided data from a lab process, previously described, performed prior to this master thesis. The lab data has been used to perform mass and balances calculations which have set a foundation for the simulation of the up-scaled process in Aspen Plus. Process integration, including heat and chemicals, have been conducted manually through different calculations. Finally, the capital and operational costs of the plant have been calculated and a break-even price of the produced pulp has been determined.

3.2.1 Mass and energy calculations

Based on lab data, mass balances were determined through implementation of equation 2.2. This was done by assuming a constant content of cellulose throughout the process and a production of 1 kg dissolving pulp. Furthermore, data of the amount of mannose, acid soluble lignin (ASL), xylose arabinose, were not consistent, which could be due to their small amounts, making them difficult to detect by the analytical instrument HPAEC (High-performance anion-exchange chromatography).

Due to the small content of mannan, ASL, xylan and arabinan in oat husks, the precision of the analytical lab analysis did not detect their monomeric form in all steps of the lab trial. Therefore, some assumptions were made for the sake of the mass balances. Firstly, when data was missing in a step, their content was assumed to remain equal to the previous step. Secondly, in a similar trial, the arabinose content after bleaching was detected as 44.7% of its content after cooking. Thereby, the same ratio was assumed to be true in the final lab trial. Finally, undetected content, not characterised by HPAEC in any step, was simplified as "others".

Based on the mass balances and additional lab data, energy balances were calculated according to equation 2.4. Due to water being by far the most predominant liquid, the heat capacity of water was used for all liquids except for hydrogen peroxide.

The mass and energy balances were later recalculated for industrial scale where the plant was assumed to be under operation 8400 hours of the year. To perform these calculations, the following assumptions regarding the availability of oat husks as raw material was made. Firstly, based on the found husk to oat ratio, the oat husks mass yield was assumed as 30% of the harvested oats. Secondly, all oat husks harvest in counties close to Nymölla in Skåne, were assumed to be sent to the plant. These counties being Västra Götaland county, Halland county, Skåne county, Kalmar county, Kronoberg county, Jönköping county and Östergötland county. The production of oat husks in these counties were estimated based on data from The Swedish Board of Agriculture's official statistics, see Table A.2.

Thereby, the amount of available raw material at industrial scale was estimated to 145 440 ton per year and the mass and energy balances could be recalculated at a larger scale.

The amounts of chemical and water in the liquors were determined in the same manner as in lab scale, and were hence, scaled up linearly, see Table 3.1.

Table 3.1: Liquor composition in lab and industrial scale, with chemicals defined as Chem. A and Chem. B and their concentrations in weight percentage.

Process step	Liquid-to-solid ratio	Chem. A	Conc. [wt%]	Chem. B	Conc. [wt%]
Prehydrolysis	6:1	HCl	0.1		
Cooking	8.3:1	NaOH	4		
Bleaching	10:1	H_2O_2	5	NaOH	0.04

This was done to ensure the same pH in industrial scale as in lab scale.

3.2.2 Simulation in Aspen Plus

The prehydrolysis soda pulping simulation was modelled in Aspen Plus software version 12.1, based on a similar flow chart as in lab scale, seen in Figure 3.1. The main difference is seen in the lack of a washing step between prehydrolysis and cooking, as these steps commonly are performed in the same digester in industrial scale. Furthermore, no defibration is simulated as this is not possible in Aspen Plus nor expected to be needed in industry.

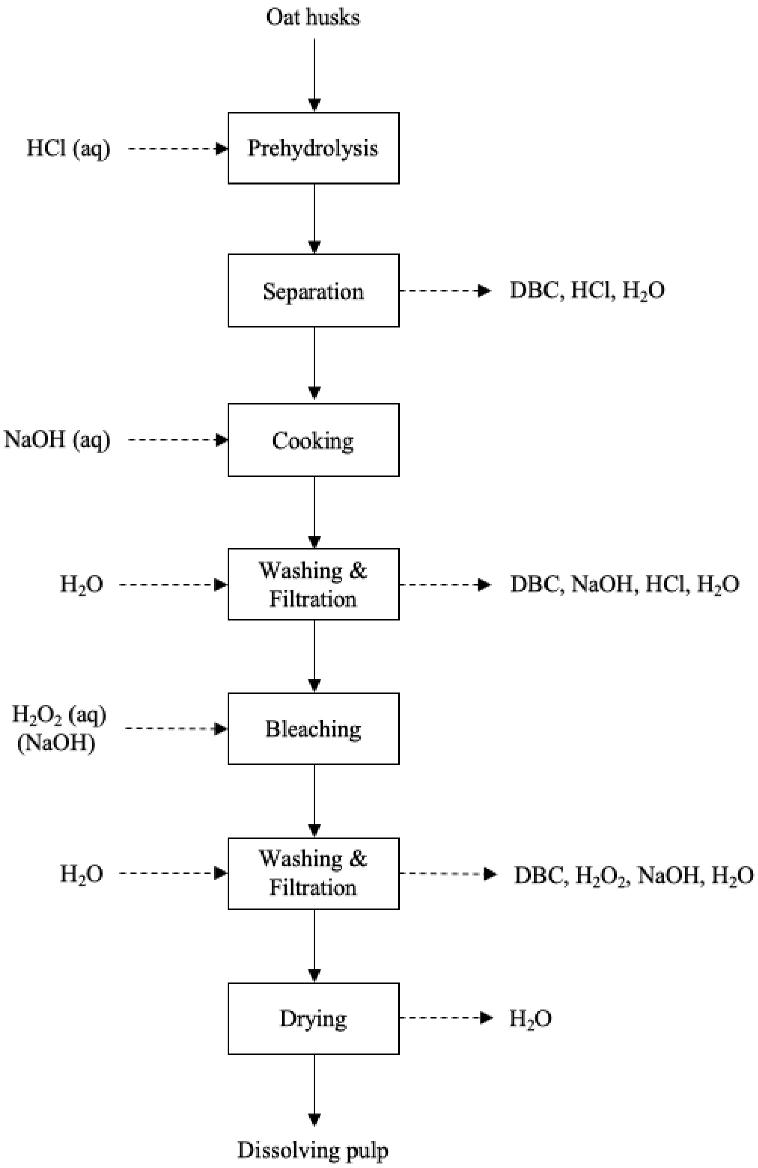

Figure 3.1: Flow chart of pulping process from oat husks to dissolving pulp with all inputs and outputs as simulated in Aspen Plus, where DBC is abbreviation for dissolved biomass components.

The biomass was characterised by specifying its different components, which all were defined as solids. Cellulose was selected from the polymer data bank and its heat of formation was specified to match the enthalpy of hydrolysis. Galactan and mannan were specified the same way as cellulose. Xylan was characterised as a user defined component and arabinan was characterised identically to xylan. Klason lignin and acid soluble lignin (ASL) were both defined as vanillin. The klason lignin was further specified in regard to enthalpy to match condensed vanillin and solid heat capacity. Ash was defined as silicon dioxide. The final components, not measurable in lab scale, were named "others" and were defined in the same way as ash for simplification.

The specifications made for cellulose, hemicelluloses and lignin are seen in Table A.3, where all constants and values were specified accordingly with *Aspen: Characterization of Lignocellulosic Biomass with Specification in Aspen Properties*, provided by Aspen Technology 2021.

The NRTL model was chosen as the base property model due to the relatively low operating pressures as well as the characteristics of the components. Since the streams in the process both will contain solids from the biomass and liquids from the added chemicals and water, the MIXCISLD stream class was selected. In the first inlet streams, the biomass components were defined as CI Solids and the water content as Mixed. In the other inlet stream, the prehydrolysis liquid, both hydrogen chloride and water were defined as Mixed components. Both inlet streams were set to a temperature of 25°C and a pressure of 1 atm. The prehydrolysis and cooking were simulated in a step-wise manner and in two main parts. First the two inlet streams were modelled to enter a mixer, then the flow was pumped to a pressure of 7 atm and heated to 160°C, before letting it enter the prehydrolysis reactor. An RStoic reactor was used to simulate the hydrolysis and dissolution of the biomass components by specifying the fractional conversions for the different components from CI Solids to Mixed. Thereafter, a component separator was used to separate 85% of the dissolved components and hydrochloric acid as well as 65% of the added water, see Table A.8 for unit settings. The amount of water to be removed was selected, throughout the simulation, to ensure a slightly higher water content in the mass flow than the previously determined water content after each treatment.

The second main part, representing the cooking, was simulated by mixing the prehydrolysis outlet stream with white liquor (WL), increasing the pressure to 8 atm by inserting a pump and heating the stream to 170°C. As in prehydrolysis, an RStoic reactor was used to simulate the hydrolysis and dissolution of the different biomass components. Thereafter, 85% of the dissolved components and sodium hydroxide was extracted from the mass stream by a second component separator, settings specified in see Table A.9, to simulate removal of black liquor. A SWash was implemented where a water flow of 35 ton per hour was pumped into the washer, with a pressure of 9 atm. The flow of the washing water was chosen to be roughly the amount of water needed to be replaced in the pulp and to be within the range of 2 to 3 tonnes per ton of pulp. Also, the water pressure was selected to avoid evaporation. Finally, the washing was finalized by an additional component separator, settings specified in Table A.10, to remove the final dissolved components, chemicals as well as the excess water.

The outlet stream was then mixed with a new inlet stream of bleaching liquor. The mixed stream was heated to 80°C and a final RStoic reactor was implemented. As after cooking, the separation and washing steps were repeated. For settings in the two washing units and the fourth separator, see Table A.13 and Table A.11. Finally, to simulate air drying of the wet dissolving pulp, the final component separator was adjusted to remove larger amounts of water, to reach the desired 50% dry content, settings presented in Table A.12.

3.2.3 Process integration

The heat integration and the recovery of chemicals were accounted for manually. The valuable black liquor, consisting of dissolved biomass components, water and chemicals from prehydrolysis and cooking, were assumed to be sent to a nearby kraft mill. In this neighbouring mill, the black liquor is directly sent to the evaporators and then the concentrated black liquor is burnt in a recovery boiler to produce steam and recover chemicals. The steam being produced in the recovery boiler of the kraft mill was assumed to be integrated with the oat pulping plant. A ΔT_{min} of 10°C was assumed and due to the temperature demand to heat the process steam in prehydrolysis and cooking, medium pressure steam was required. The heat load of the MP steam produced in the recovery boiler was determined as

$$Q_{steam} = m_{steam} \cdot L \tag{3.1}$$

where the m_{steam} represents the mass of steam and L the latent heat of vaporisation. As MP steam was to be produced, leatent heat of vaporisation at 10 bar and 180°C, of 2776 kJ/kg, was implemented [28].

Of the sodium hydroxide available in the black liquor, 80% was assumed to be recovered by the kraft mill, due to the efficiency of the causticizing reaction, see section 2.3.5. As one does not wish to enter chloride into a kraft mill, sulphuric acid was considered to replace hydrochloric acid in the prehydrolysis. Both the sulphuric acid and the sodium hydroxide was assumed to be reused in the kraft mill, as make-up chemicals. The excess water in the black liquor was assumed to be handled in the evaporation plant, prior to the recovery boiler.

3.2.4 Adjustments for a sulphuric acid prehydrolysis

Prior to the cost evaluation and environmental assessment, new calculations based on new lab data, where sulphuric acid was used as prehydrolysis chemical instead of hydrochloric acid, was performed. The total amount of dissolved components was determined based on the composition of the raw material and the final product.

No modelling of a sulphuric acid prehydrolysis was performed. Instead, the composition and amounts of different output streams were determined manually. Firstly, based on the previously determined input of sulphuric acid, 85% of this was assumed to end up in the black liquor, while the amount of sodium hydroxide in the black liquor was kept the same as in the modelled process. To determine the content of dissolved components in the black liquor, the same ratio as in the modelled process was implemented. In similar to the content of dissolved components, the amount of water in the black liquor originating from prehydrolysis, was defined as 66.9% of the input of water in the liquid in the prehydrolysis, since this was the case in the modelled process. The amount of water from cooking to the black liquor was kept the same as in the modelled process. The total amount of water in all output streams, besides in the dissolved pulp, was assumed to be reduced by 32.24 kg per hour, due to this decrease of water in the prehydrolysis liquor.

3.2.5 Cost evaluation

Capital costs, such as the cost of different process equipment, were estimated due to large price fluctuations and difficulties to find consequent data, see Table A.18. The process was assumed to have a need of four batch digesters, three bleaching stages, two washers and twice as many pumps as needed to run the process. In this case, the cost estimation of washers considered also the filtration of waste liquors. Even though screening equipment was not accounted for in the simulation of the process, it was accounted for in the economical assessment, to cover a possible need at industrial scale. The cost of the three heat exchangers were determined based on the equations 2.5, 2.6 and 2.7, whereof U was estimated as 1500 W/m2°C based on data for similar streams found in *Chemical Engineering Design* by R. K. Sinnott and G. Towler, 2013. Finally, CAPEX was determined as the total expected capital costs.

Operating costs, however, were calculated based on data seen in Table A.19. The cost of chemicals being based on SCB's foreign trade statistics. The cost of process water was estimated based on recommendations in *Chemical Engineering Design* by R. K. Sinnott and G. Towler, 2013. The electricity cost was determined based on the electricity price in south of Sweden in May 2022. The fixed operating costs covered wages, supervision, management, maintenance, insurance and taxes. These were all calculated based on a few assumptions, all summarised in Table A.20. Furthermore, some of both the sodium hydroxide and sulphuric acid were assumed to be sold to a kraft mill with zero profit. The chemicals lost within the system were assumed to be completely financed by the oat pulping plant alone. The cost of oat husks, since it is often used for energy purposes, was estimated based on the assumption to be sold to a similar price as forest residues for fuel applications.

Excess steam from the black liquor was assumed to be sold to the grid, which was included as a yearly income in the economic assessment. The income was estimated by assuming an income equal to the avoided cost of electricity.

Finally, the break-even price was determined by assuming full production already during the first year and a full payback of capital costs within the first three years.

3.3 Results

The results from the techno-economic assessment are presented in this section. This includes the simulation in Aspen plus, the different input and output flows and heat demands, as well as the process integration and cost evaluation.

3.3.1 Process simulation

In industrial scale, an input of 17.3 tonnes of oat husks per hour will result in an hourly production of 9.8 tonnes of dissolving pulp with 50% water content, which makes a dry weight of 4.9 tonnes and an efficiency of 28.3%. A detailed composition of the dissolving pulp is found in Table A.17. The ratios of the dissolving pulp components are, as seen, the same as in lab scale and this is also true for the different process temperatures. In Table 3.2, the chemical requirements per ton of wet pulp (50% water content) are presented, under the assumption that no chemicals are recirculated within the oat pulping plant.

Table 3.2: Total input of chemicals per ton of wet pulp (50% water content).

Chemical	[kg/ton wet pulp]
Sulphuric acid	13
Sodium hydroxide	368
Hydrogen peroxide	254

The highest chemical demand is, as seen, of sodium hydroxide, closely followed by hydrogen peroxide. In the tree liquors, the total water requirement sums up to 16.8 tonnes. The hourly input of the three process liquors are presented in Table A.14 - A.16.

The process modell, created in Aspen Plus, is presented in a step-wise manner in three different figures, where Figure 3.2 is a presentation of the simulated prehydrolysis. An overview of the entire process as simulated in Aspen Plus is found in Figure A.2.

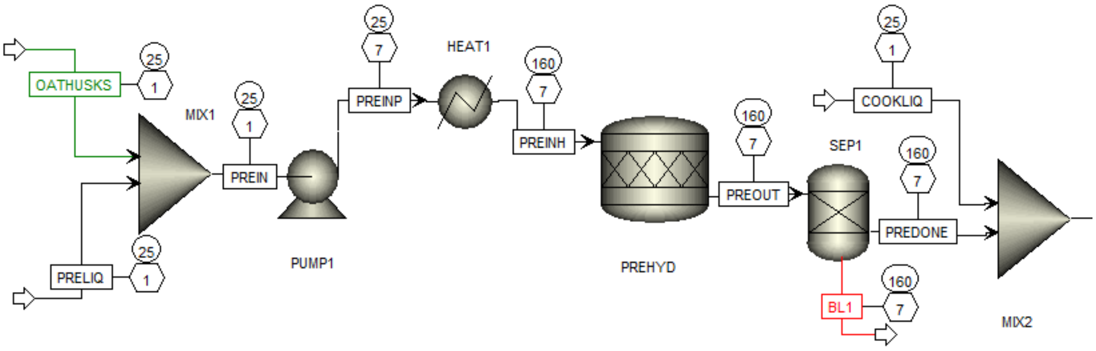

Figure 3.2: Model of prehydrolysis in Aspen Plus. Name of units specified above or below, name of flows in rectangles, temperatures (°C) in circles and pressures (bar) in hexagons.

The model, seen in Figure 3.2, describes an input of oat husks and prehydrolysis liquor, two output - one of black liquor (red arrow) and another of prehydrolysed mass. For clarification of the different flows, see Table A.5.

The second part of the model includes the cooking process as well as washing and separation, see Figure 3.3.

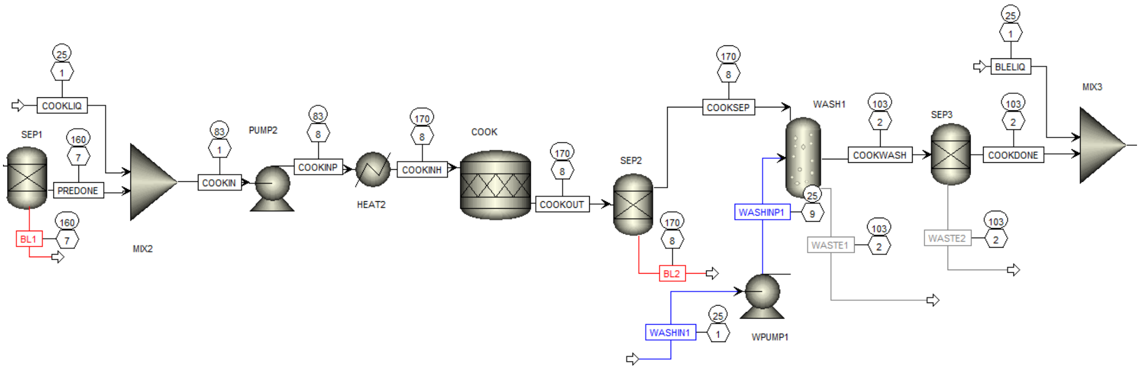

Figure 3.3: Model of cooking and washing in Aspen Plus. Name of units specified above or below, name of flows in rectangles, temperatures (°C) in circles and pressures (bar) in hexagons.

The cooking model visualises an input of prehydrolysed mass, from the prehydrolysis, and of white liquor (WL). As can be seen, four outputs are modelled - black liquor (red arrow), two waste streams during and after washing and the pulp. The two residue streams (grey arrows) are in reality only one but are modelled as two in Aspen Plus. The blue arrows represent flows of washing water. In Table A.6, all different flows seen in Figure 3.3 are defined.

In Figure 3.2, the third and final part of the model, representing the bleaching and the final washing, separation and drying of the dissolving pulp, is presented.

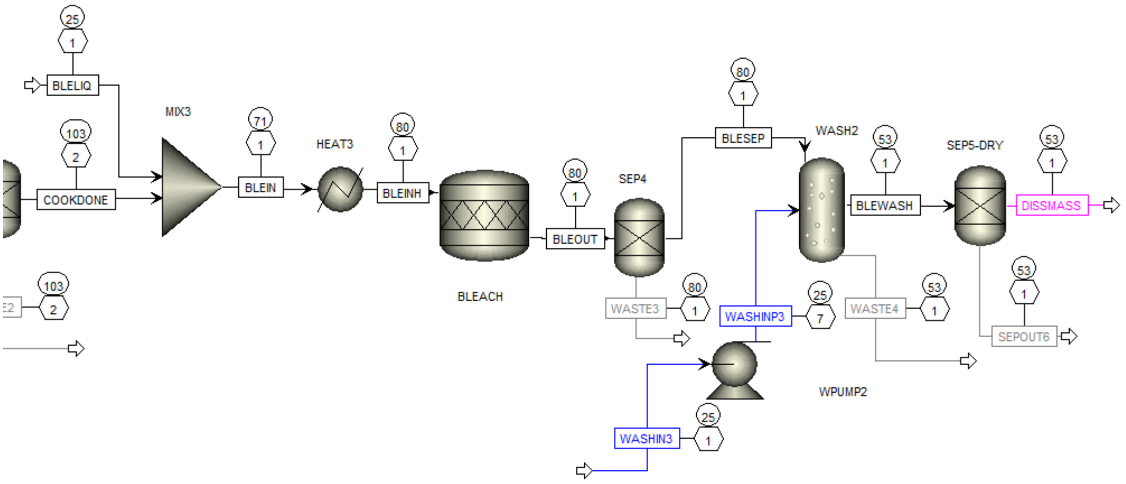

Figure 3.4: Model of bleaching and washing in Aspen Plus. Name of units specified above or below, name of flows in rectangles, temperatures (°C) in circles and pressures (bar) in hexagons.

In similar to the cooking model, the simulation of bleaching contains two inputs and four outputs. One input of pulp and one of bleaching liquor. Blue arrows represent the flow of washing water and the grey arrows, the two residue flows. Finally, the lilac arrow represents the final output - from the bleaching and from the entire pulping process - dissolved pulp. The produced wet dissolving pulp has 50% dry content and 50% water content.

A list and description of the different process units, as seen in Figure 3.2 - 3.4, are found in Table A.4.

The heat requirements for the three key process steps, prehydrolysis, cooking and bleaching, are seen in Table 3.3, along with the electricity requirements for the pumps.

Table 3.3: Heat and electricity requirements in the pulping process.

Process step/unit	Type	Demand [kW]
Prehydrolysis	MP steam	16461
Cooking	MP steam	10172
Bleaching	MP steam	516
Pumps	Electricity	45

As can be seen, the highest heat demands originates from prehydrolysis and cooking, as these require the highest temperature increases. Bleaching occurs at a lower temperature, of in which LP steam could be used instead of MP steam. However, MP steam is chosen to heat all parts of the process both due to simplicity in steam production and as this will lead to a lower area requirement in the heat exchanges, and hence, lead to a lower capital cost. The electricity requirements for the pumps are, in comparison, quite low.

The two washing steps requires 35 tonnes and 29 tonnes of water per hour, respectively, which gives a demand of 6.6 tonnes washing water per ton wet pulp. The time demands for the different steps are not covered in the process simulation in Aspen Plus.

3.3.2 Heat and chemical integration

In the recovery boiler, MP steam with a heat load of 34.8 MW is produced, which covers 128% of the heating demand of the oat pulping process. Thereby, the entire heating demand of the process is covered by the integrated steam and excess steam, of 7.6 MW, can be sold to the grid.

As 80% of the sodium hydroxide in the black liquor from the oat pulping plant enters the kraft pulping process, the kraft mill's demand of sodium hydroxide would be fully covered. In fact, the oat pulping plant would likely provide the kraft mill with more sodium hydroxide than could be handled. Assuming a softwood kraft mill, with a fresh sodium hydroxide input requirement of 25 kg per Adt softwood pulp, the kraft mill would need to have a yearly production of 1.2 million Adt pulp to handle all sodium hydroxide.

The large amounts of sodium hydroxide delivered from the oat pulping plant to the kraft mill, is in line with no recirculation within the oat pulping plant. The high fresh input of 368 kg sodium hydroxide per ton wet pulp in the oat pulping process is, thus, translated to 662 kg NaOH per Adt.

3.3.3 Costs

In Table 3.4, the expected capital costs for the plant are presented, including cost estimations of process equipment, calculated costs for the three heat exchangers and CAPEX.

Table 3.4: Capital costs in year 2022 with an annual production capacity of 45 443 Adt dissolving pulp.

Capital costs	[SEK]
Stepwise batch digesters	400 000 000
Bleaching equipment	240 000 000
Washers	100 000 000
Screener	30 000 000
Pumps	600 000
HX Prehydrolysis	24 648
HX Cooking	25 585
HX Bleaching	10 298
CAPEX	770 660 523

The process equipment is, thus, calculated to include four digesters, three bleaching stages, two washers, one screener, eight pumps and three heat exchangers. CAPEX is, thus, determined to approximately 771 MSEK.

A part of the sodium hydroxide and sulphuric acid input will be sent to the neighbouring kraft mill, and thus, allocation of the operating cost for these chemicals results in the following operating costs, seen in Table 3.5. The operating costs are determined based on the assumption that the shared chemicals will be sold to the kraft mill with a zero profit while the chemicals being lost as waste within the system are to be financed by the oat pulping plant.

Table 3.5: Operating costs in year 2022 with an annual production capacity of 45 443 Adt dissolving pulp.

Operating costs	[SEK/year]
Oat husks	465 408 000
Sodium hydroxide	265 576 730
Sulphuric acid	386 884
Hydrogen peroxide	82 511 623
Process water	44 087 330
Electricity	1 043 124
Fixed operating costs	[SEK/year]
Wages	9 135 000
Supervision	1 827 000
Management	4 567 500
Maintenance	38 533 026
Insurance	7 706 605
Taxes	15 413 211
OPEX	936 196 034

As can be seen in Table 3.5, OPEX is approximately 936 MSEK per year.

In addition to the expected yearly costs, a yearly income is expected from the excess steam, which is to be sold to the grid. The excess steam, thus, provides a yearly income of approximately 80.87 MSEK. Thereby, the break-even price of the dissolving pulp becomes approximately 14 322 SEK per ton of dry weight pulp.

4

Environmental assessment

4.1 Goal and scope definition

The goal of the environmental assessment is to predict the main environmental impacts associated with the production of dissolving pulp with oat husks as raw material. This is to be assessed in a prospective life cycle assessment, from cradle to gate.

The process to be investigated in this prospective LCA is the one investigated in the techno-economic assessment and modelled in Figure A.2, where oat husks are treated in a prehydrolysis soda pulping process to form dissolving pulp. The functional unit of this assessment is defined as 1 ton of wet dissolving pulp. The reference flow is, thus, 1 ton of wet dissolving pulp - with 50% dry content and 50% water content. The assessment will investigate the environmental burden connected to the pulping process. Some impacts on the energy system will also be accounted for, as the excess energy, produced as steam in the recovery boiler of the neighbouring kraft mill, will be sold to the grid. The oat pulping plant will, through mass allocation, be held accountable for part of the environmental burden from the sodium hydroxide and sulphuric acid, since these are sent to and used in the neighbouring kraft mill. More precisely, for the chemicals being used in both plants, the burden will be divided equally. However, the oat pulping plant will also be held accountable for the chemicals being lost in the oat pulping process and in the recovery boiler of the kraft mill. The oat husks being a residue from agriculture, will not be assessed to hold any environmental burden within the system.

The assessment will, hence, focus on the possibility of using oat husks as raw material for the production of dissolving pulp. Thereby, the extraction of oat husks form other areas of application and how these system may be impacted by this, will not be covered in the assessment.

The assessment will be performed based on data provided from the previously performed technical assessment, where the process has been modelled in industrial scale. Required data, not provided by the technical assessment, will as far as possible be collected from the GaBi database Sphera. When needed, scientific articles will be used as reference.

4.1.1 System boundaries

As the impact from the oat production will not be accounted for, the technical system will be limited by the production of dissolving pulp. The model will, hence, include the process of dissolving pulp production, beginning with the transport of oat husks and chemicals to the plant and ending with the product, wet dissolving pulp. The steam production in the neighbouring kraft mill will also be included in the model, whereof only the burden from the produced steam, which will be integrated with the oat pulping plant, is accounted for. The burden from the excess steam production will be excluded from the system and, instead be associated with the kraft mill. The new, additional input of electricity, from the excess steam, to the grid will be handled as a credit. The credit describes a reduction in previous electricity production, being linear with the input of excess steam. When no burden of the excess steam production is included in the credit, this is later described as "avoid. el.". Additionally, the burden for waste water treatment of the waste flows not sent to the kraft mill, will be included within the system.

The location of the plant will be in Skåne, and the oat mills, providing the oat husks to the plant, are geographically limited to south of Sweden. However, as the chemicals are assumed to be provided from other countries in Europe, the geographical boundary of the system will be expanded to Europe. The time perspective considered in this assessment is 10 years. The time horizon is chosen to cover both the production of dissolving pulp from oat husks as well as the consequences of the process.

4.1.2 Environmental impact categories

The main impact category of interest in this assessment can be argued to be global warming potential, GWP, since it provides a clear indication of the expected climate change owning to the system. GWP considers greenhouse gas emissions, in CO_2 equivalent, and gives an indication of the ecological consequences of the system [29]. GWP biogenic carbon is excluded from the assessment in GaBi. In addition to climate change, acidification, eutrophication, abiotic depletion and photochemical oxidation formation are of high interest. The five parameters are selected to cover different sorts of categories, which are expected to have high burdens from chemical production, as these processes are expected to be of higher burden to the system. As a energy credit is considered in the system, the total use of renewable primary energy source and non-renewable primary energy sources are too of high significance.

All investigated categories and their respective parameters are listed in Table 4.1.

Table 4.1: The impact categories and their respective parameters.

Impact category	Parameter
Global warming potential - fossil fuels	GWP (fos)
Global warming potential - land use and land use change	GWP (lnd)
Global warming potential - total	GWP (tot)
Acidifiation potential	AP
Eutrophication potential	EP
Photechemical oxidant formation	POF
Abiotic depletion (ADP elements)	ADP
Total use of renewable primary energy resources	PERT
Total use of non-renewable primary energy resources	PENRT
Use of net fresh water	FW
Hazardous waste disposed	HDW
Non-hazardous waste disposed	NHWD
Radioactive waste disposed	RWD

The associated impact assessment method for each impact category are listed in Table B.6.

4.2 Method

The LCA has been conducted in the software GaBi, where the pulping process has been modelled by defining its required inflows and outflows, see Figure B.1. For each inflow, such as sodium hydroxide or electricity, a process has been selected to cover the burden from it, see Table B.1. All inflows which require transportation to the plant were assigned a transportation process, chosen based on whether the production site being assumed to be within Sweden or somewhere else in Europe. The distance for transportation of oat husks was defined as the average distance from the oat mills, delivering the oat husks. A transportation process with a fuel mix likely to be used in Sweden was chosen for this transportation, since it was to take place within Sweden. The chemicals, on the other hand, were assumed to be produced outside of Sweden, somewhere in Europe. A distance of 1500 km was estimated and a transportation process with a lesser ratio of biofuel was chosen. The load factor for all transportation were set to 0.85, by default. See Table B.2 and Table B.3 for defined transportation processes and settings.

From the pulping process, three flows were defined as outputs - the dissolving pulp, waste liquor to the kraft mill and waste water. The waste water was modelled to be sent to a waste water treatment process and the waste liquor was modelled to produce steam in three steps. First, the waste liquor, or weak black liquor, was modelled as an inflow and black liquor as an outflow. Secondly, the black liquor was divided into two streams - one which would become steam to be used in the oat pulping plant and another to become steam to be sold to the grid. The first stream of black liquor was modelled as an inflow to a steam production process, which was created manually. The process for steam production was created to resemble one of fuel production from forest residues, by specifying the emissions seen in Table 4.2 as outflows. The emissions were determined based on data seen in Table B.4.

Table 4.2: Emissions from steam production accounted for by the oat pulping plant.

Emission	kg/h
Carbon dioxide	185.703
Methane	0.014
Nitrogen oxides	1.173
Nitrous oxide	0.006
Sulphur dioxide	0.041

The steam, which exited this process, was defined as the steam to be sent back to the oat pulping plant to cover its heating demand. The second stream of black liquor was also modelled to be processed in to steam in a similar process, based on the same emission data. However, these emissions were not considered to be caused by the oat pulping plant and where, hence, assigned to the kraft mill. Furthermore, the outflow of steam was modelled as a credit, where the energy provided by the excess steam led to the same decrease in electricity. Thereby, a reduction of electricity was modelled and the gain from this reduction was assigned to the oat pulping plant and the system.

For further investigation of the energy credit, a second model was created, where electricity was exchanged into natural gas.

4.2.1 Mass allocation

In the software GaBi, the burden from each modelled process was determined for the different impact categories. The burden from two of the three chemicals, sodium hydroxide and sulphuric acid, were allocated between the investigated system and the other system, the kraft mill. Mass allocation was performed and the calculations are seen in equation B.1 and equation B.2, see Table B.7 for data. The mass allocation was implemented in the processes of chemical production and transportation.

4.2.2 Sensitivity analysis

To test the robustness of the assessment, a sensitivity analysis was performed. The sensitivity analysis was performed by allocating the burden of the chemicals differently, by only allocating the burden of the lost chemicals to the oat pulpng plant and all burden from the reused chemicals to the kraft mill, see Table B.8 and equation B.3. Thereafter, the climate impact associated with drying the pulp was estimated based on GWP from electricity production, an evaporation energy of 2 263 kJ per kg of water for drying of wet pulp as well as an estimated heat recovery efficiency of 50%.

Finally, since no GWP biogenic carbon is accounted for in the assessment, an estimation of its burden due to steam production in the recovery boiler was roughly estimated based on the lower heating value of wheat straw lignin content, of 20.15 MJ/kg wt% (dry basis) [30]. This was done based on all steam produced in the recovery boiler, including both the excess steam and the steam integrated with the oat pulping plant.

4.2.3 Normalisation

Finally, five of the assessed impact categories were subjected to normalisation based on global reference values from IVL database, see Table B.5, to identify the impact category with the highest burden.

4.3 Results

In this section, graphs are presented to visualise the results from the environmental assessment. Four different cases are presented, whereof Case B (avoid. el.) represents the case as defined as in goal and scope. Case A (no credit), represents a simplified scenario, excluding any energy credit while Case C (SA avoid. el.) and D (SA credit), are part of the sensitivity analysis. Finally, graphs to compare the four cases are presented. A list of the names used for the different processes in the graphs is seen in Table B.9

The firs case to be presented is Case B, since it represents the system as described in the goal and scope, section 4.1, and includes the reduced impact due to avoided electricity production. The climate impact of Case B is determined to 558 kg CO_2-eq/ton wet pulp, excluding biogenic carbon. An overview of the contribution to the burden of all investigated categories is presented in Figure 4.1. The contribution from each process is visualised in percentage.

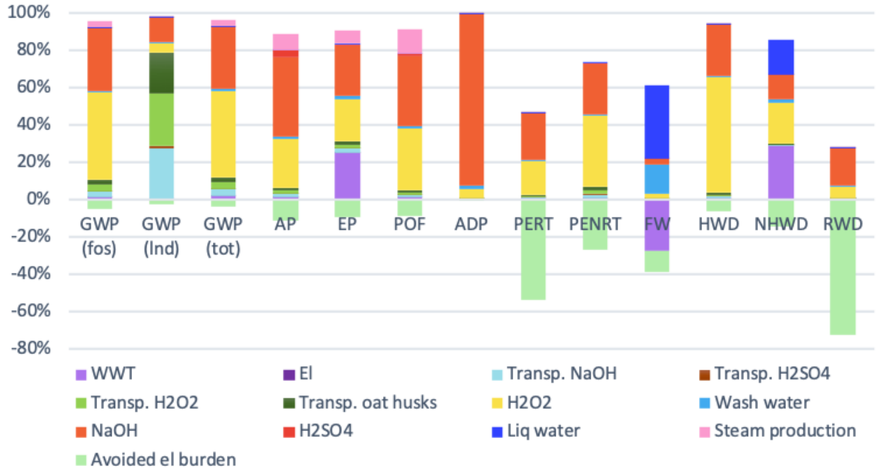

Figure 4.1: Case B (avoid. el.) - percentile distribution of the burden in all processes and all assessed impact categories.

As visualised in the graph, the sodium hydroxide and hydrogen peroxide production are responsible for a greater part of the burden in the majority of the impact categories. Furthermore, the transportation of raw materials holds all together just below 80% of the GWP (lnd) Most negative burdens are caused by the avoided electricity burden, originating from the energy credit, and this is seen to have the greatest impact on on PERT and RWD. A graph, where only the five selected impact categories are investigated, is seen in Figure B.2.

The reduced burden due to the energy credit, in Case B, is further investigated in Figure 4.2, where the choice of energy to be replaced by the excess steam is assessed. Here, the reduced burden from avoided electricity production is compared to the reduced burden from the same load of avoided natural gas.

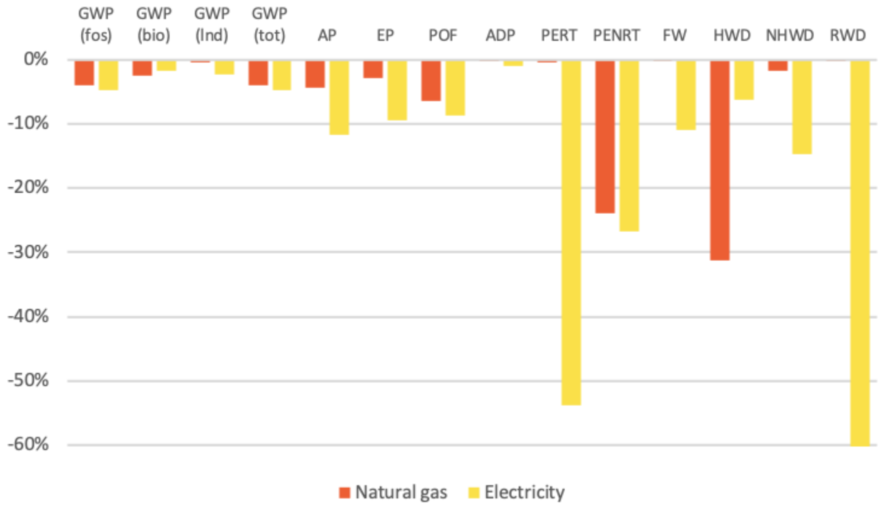

Figure 4.2: Percentile comparison of avoided burden from a natural gas credit and electricity credit.

The negative staples in the graph indicate reduced burdens when the excess steam replaces natural gas or electricity. The reduced burden is, thus, seen to be similar in most categories regardless if electricity or natural gas is replaced by steam. Electricity, however, shows a great negative burden in PERT and RWD, while close to no reduction is seen in these categories for natural gas. Natural gas, however, has a considerably greater negative burden in HWD than electricity.

A similar graph to Figure 4.1, presenting a case where no avoided electricity burden is included in the system, is seen in Figure B.3. This case is defined as Case A, since this scenario includes less processes and is in some way a simplification of the Case B. By comparing these two cases, seen in Figure 4.1 and Figure B.3, the sodium hydroxide and hydrogen peroxide are seen to be assigned even greater parts of the burden of the system, when no avoided electricity production is included. The greatest change is seen in PERT and RWD, which were mostly affected by the avoided electricity burden, where the two chemicals have increased their total burden from approximately 40% and 30%, respectively, to over 90% in both categories. Additionally, the climate impact, excluding biogenic carbon, is increased to 588 kg CO_2-eq/ton wet pulp.

4.3.1 Sensitivity analysis

In the following graph, seen in Figure 4.3, a similar scenario to Case B has been analysed. In this case, Case C, the system is similar to Case B, but the allocation of the burden from sodium hydroxide and sulphuric acid have been handled differently. Case C, hence, represents a case where the burden from these two chemicals have been reduced, as the system only accounts for the chemicals being lost as waste, and none of the chemicals being shared by the oat pulping plant and the kraft mill. This, hence, leads to a reduction to 441 kg CO_2-eq/ton wet pulp in climate impact, excluding biogenic carbon.

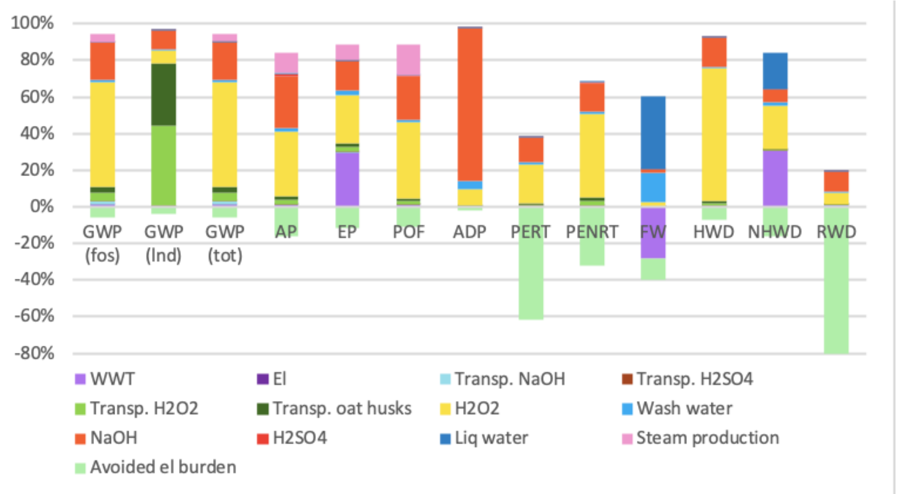

Figure 4.3: Case C (SA avoid. el.) - percentile distribution of the burden in all processes and all assessed impact categories.

As can be seen, when comparing Case C to Case B, the percentile distribution of the burden originating from sodium hydroxide is affected. As the burden from the sodium hydroxide process is decreased, the burden of the hydrogen peroxide process is assigned a larger percentage of the total burden in most impact categories. As the burden from sulphuric acid already was quite low in Case B, its burden is hardly visible in Case C.

The final case, Case D is presented in Figure B.4. This case is almost identical to Case C, but also includes the burden from the excess steam production. This burden is not included in the other cases, since it is defined to relate to the kraft mill and not the assessed system. However, Case D is of interested to the assessment to investigate how this system boundary affects the system and is seen to have a climate impact of 446 kg CO_2-eq/ton wet pulp.

By comparing Figure 4.3 to Figure B.4, no drastic changes are detected. Case D is seen to have a slightly higher climate impact, excluding biogenic carbon, than Case C. Furthermore, slight increases in AP, EP and POF are detected, whereof, the largest increase is seen in POF.

In no cases, drying of the pulp has been included in the assessment. This is why all results are presented per ton of wet dissolving pulp. The climate impact for drying, excluding biogeninc carbon, was estimated to 58 kg CO_2-eq/ton wet pulp. The climate impact for the four cases, in alphabetic order, could hence be estimated to 1233, 1174, 939 and 950 kg CO_2-eq/ton dry pulp, respectively. Lastly, GWP biogenic carbon, from the steam production of all steam, was roughly estimated to 1065 kg CO_2-eq/ton wet pulp.

4.3.2 Comparison of the four cases

The four previously presented cases shows different burdens in regard to climate change. The burden of the three impact categories representing climate change are, thus, compared for the four different cases in kg CO_2-eq/ton wet pulp in Figure 4.4.

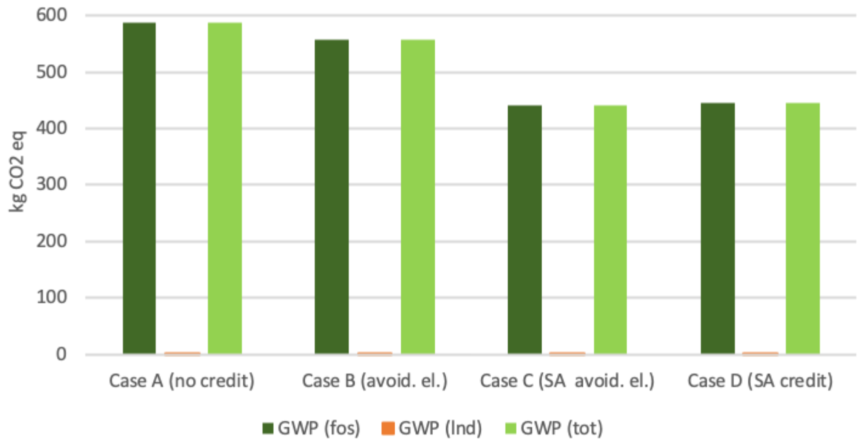

Figure 4.4: GWP (fos), GWP (lnd) and GWP (tot) for Case A (no credit), B (avoid. el.), C (SA avoid. el.) and D (SA credit) in kg CO_2-eq/ton wet pulp.

Case A, where no reduction of burden is considered as a cause of the sold excess steam, have the highest values for GWP (fos) and, consequently, also GWP (tot). As can be seen, from Case A to Case B, these impacts are slightly reduced from 587 and 588 to 557 and 558 kg CO_2-eq/ton wet pulp, respectively. The largest deviation is, however, found for Case C and D, where the climate impact is noticeably reduced in comparison to Case A and B. Case C and D are, though, close to identical in terms of GWP. For both Case C and D, GWP (fos) and GWP(tot) are approximately 450 kg CO_2-eq/ton wet pulp. In all cases, GWP (lnd) hold a very low burden.

A similar comparison is seen for PERT and PENRT for the four cases in Figure 4.5, where the burdens are presented in MJ/ton wet pulp.

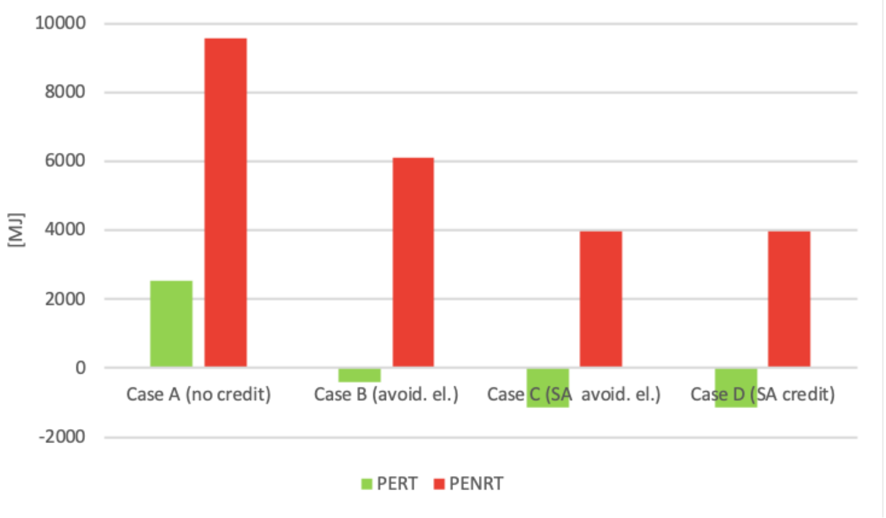

Figure 4.5: PERT and PENRT for Case A (no credit), B (avoid. el.), C (SA avoid. el.) and D (SA credit) in MJ/ton wet pulp.

Case A indicates a high burden of PENRT and, in comparison to the other cases, a high burden of PERT, as well. The second highest burden of PENRT is seen in Case B. In Case C and D, PENRT has been reduced by 2000 MJ and in all three of these final cases, PERT has a negative value, whereof the lowest values are found in Case C and D.

To put the impacts of climate change, acidification, eutrophication, abiotic depletion and photochemical oxidant formation into context, a graph presenting the normalised values for the four cases is viewed in Figure 4.6.

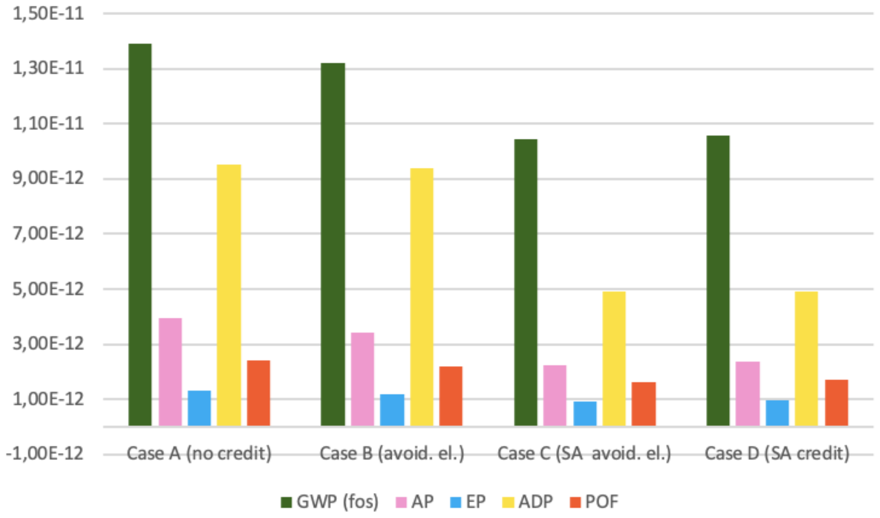

Figure 4.6: GWP (fos), AP, EP, ADP and POF per ton of wet dissolving pulp normalised to global reference values for Case A (no credit), B (avoid. el.), C (SA avoid. el.) and D (SA credit).

The graph has been normalised to global total impact values and in all four cases, GWP (fos) can be seen to be the most critical impact category with the highest impact. The second most critical impact category is seen to be abiotic depletion, which is then followed by acidification, photochemical oxidant formation and lastly, eutrophication. Furthermore, Case A provides the highest burden in all five categories and Case C and D, the lowest. GWP (fos) is seen to be the impact category whose burden is reduced the most from Case A to Case B, while the other burdens are just slightly reduced.

5

Discussion

The simulation of the oat pulping process in Aspen Plus can be seen as the life cycle inventory of the project. As the composition of the different output streams are determined in the simulation as well as the heat demand of the different process units, the simulation lays a foundation for the following tasks. The input of chemicals, seen in Table 3.2, were linearly upscaled - along with the oat husks - to ensure the pH to remain the same as in the lab trials. As no chemical recovery was included in the simulation, the simplification to instead send the black liquor to a neighbouring kraft mill for reuse there, made the input of chemicals in the oat pulping plant remain high at all times. Consequently, the plausibility of the size of the chemical inputs are difficult to justify. However, if the sodium hydroxide in the black liquor is recycled within the oat pulping plant itself, this would lead to a fresh demand of 132 kg per Adt. In comparison to a softwood kraft mill, with a fresh sodium hydroxide requirement of 25 kg per Adt, the fresh sodium hydroxide requirement in the oat pulping plant would still, however, be approximately 5 times higher. Thereby, the chemical input in the process is suspected to be higher than expected. Consequently, the size of the neighbouring kraft mill needs to be quite large to handle all the additional chemicals, as recirculation already is performed within the kraft mill itself and the demand for additional chemicals is low.

Before settling the plausibility of the size of the chemical inputs, some additional factors need to be considered. First off, the simulation was performed by specifying inputs and outputs in kg/h. The size of the reactors and, thus, the time requirement of the different step has not been specified further in the simulation. Large reactors and longer times are assumed to be required in industrial scale than in lab scale and by prolonging e.g., the cooking time, the conditions will become harsher. Furthermore, the different process steps have been simulated to occur at increased pressures, which also makes the conditions harsher and hence, the harsher conditions are expected to allow a reduction in chemical inputs. To what extent the chemical demand could be reduced is, however, difficult to estimate and therefore, this was not considered in the techno-economic assessment nor in the environmental assessment. In addition to the expected harsher conditions, one could speculate in the correctness of the assumption regarding the waste stream content. In the simulation, 85% of the sodium hydroxide and sulphuric acid input was assumed to end up in the black liquor, since some were assumed to be captured in the mass until washing. If this ratio is increased, more chemicals could be recirculated and the demand of fresh chemicals would be reduced. To truly settle how large of a chemical input to be required in industrial scale, trials with increased pressures and times, or simulation in another software is required.

Sodium hydroxide is expected to be the chemical with highest operating cost and of all operating costs, the second highest. From discussion with industry, a market price of around 10 000 SEK per ton of dry weight pulp was indicated. The break-even price as presented in the result, of 14 322 SEK per ton of dry weight pulp, is, thus, slightly higher than desired. However, if the requirement of chemicals would be reduced, which is expected, OPEX would be reduced as well and consequently, also the break-even price of the dissolving pulp. Important to note is, though, the capital cost being rough estimations, which are expected to vary greatly. Furthermore, the operating costs are calculated based on many assumptions and thus, the calculated OPEX and CAPEX should be viewed as indicators of the expected costs and nothing else. The same is to be said regarding the yearly income due to sold steam to the grid, which is an estimation and might vary depending on the actual price of MP steam.

In the environmental assessment, using the techno-econmic assessment as a life cycle inventory, the highest burdens are once again found to be caused by the chemicals sodium hydroxide and hydrogen peroxide, see Figure 4.1. Besides these two chemicals, some burden is seen to be due to the waste water treatment, the transportation of raw materials, liquid water and steam production. The other processes have a very small contribution to the environmental burden of the system. Thereby, as the chemical inputs possibly could be reduced, the burden in most impact categories and, thus, the entire system would too.

The environmental assessment also presents slightly different climate impacts for the investigated cases. In Case B, this is seen to be 558 kg CO_2-eq/ton wet pulp, excluding biogenic carbon. Case B is argued to be the scenario representing the environmental performance of dissolving pulp, produced from oat husks, most accurately. This is argued since Case B divides the burden from the shared chemicals equally between the system and the kraft mill, while all waste chemicals are accounted for by the system, as well as accounts for an electricity reduction, due to the excess steam being sold to the grid. However, one could argue that if the burden of the avoided electricity burden is included in the system, so should the consequences of extracting oat husks from an already existing heat and power plant. Case A, on the other hand, is argued to represent a scenario where too high of a burden is associated with the dissolving pulp, since no changes in the energy system is accounted for at all. However, the burden of Case A is just slightly higher than Case B, which strengthens the plausibility of Case B providing a reasonable and justified image of reality within the scope of the assessment.

In the sensitivity analysis, the choice of mass allocation method is seen to have an impact on the calculated burden. As expected, the environmental burden of the system is decreased when less burden associated to the chemicals are assigned to the system. This could be seen as a reasonable way of allocating the burden, by arguing that the neighbouring kraft mill would already be running and thus, already be assigned the burden from these shared chemicals. However, since this would result in such improved environmental performance of the system, this is not argued to justly represent reality, as it might risk indicating a too small of a burden assigned to the system. Furthermore, as seen in Figure 4.2, which type of energy too be reduced due to the added steam to the grid, has an impact on the avoided burden in the different impact categories. However, if natural gas or electricity production is reduced would in total provide a similar effect in environmental performance. One of the largest differences is seen in the total use of renewable primary energy sources, which is expected as electricity is the only alternative of these two, which uses renewable primary energy sources.

Climate impact was seen to be the most critical parameter for the environmental performance of the pulp, see Figure 4.4. Thereby, a comparison to different kind of pulps would improve the comprehensibility of the results. A common climate impact of different pulps are according to IVL estimations around 200-1000 kg CO_2-eq/ton pulp, excluding biogenic carbon. However, since no drying is included in the assessment, a comparison to other pulps is difficult. For a rough comparison, the estimated climate impacts per ton of dry pulp could be used. The estimated climate impact per ton of dry pulp in Case A and B showed a slightly higher GWP than the compared pupls, while Case C and D showed a GWP within the compared interval. This indicates a slightly higher climate impact of oat husk dissolving pulp in comparison to wood-based pulps, unless it would be decreased by a reduction in chemical demand.

Lastly, GWP biogenic carbon from steam production in the recovery boiler was roughly estimated to 1065 kg CO_2-eq/ton wet pulp. Whether or not GWP biogenic carbon should be included in an assessment is largely debated, but if so, it would increase the climate impact quite a lot.

5.1 Suggestions for future research

Many assumptions have been made throughout this thesis, whereof some might be possible to avoid by additional analyses in lab. One of the first assumptions stated, is the cellulose content being constant throughout the pulping process. In reality, a very small portion of the cellulose will be hydrolysed, and thus, the content will not remain constant. Analyses to determine the exact content in the black liquor could also provide interesting data for chemical and heat recovery.

One of the most challenging parts of this thesis, turned out to be the simulation in Aspen Plus. As Aspen Plus is not a software created to model pulp and paper processes, the process had to be simulated in a step-wise manner and with other process units than what is actually used in industry. This affected the thesis mainly regarding the black liquor and the chemicals. The amount and composition of the black liquor to be filtered from the pulp could not be determined by the software and were hence, estimated. The chemical recovery was not possible to simulate in the model and thereby, the simplification of sending the black liquor to a neighbouring kraft mill had to be done. Finally, the pH could not be measured in this process, as all components had to be specified and defined specially for this process, which is the reason why the chemical inputs were handled linearly in the scale-up. Consequently, by modelling the pulping process in a software created for pulp and paper, many of these obstacles could possibly be avoided and the simulation would possibly provide data even closer to reality, which as a consequence would have an impact on both the economic and environmental assessment.

The environmental assessment performed in this thesis strictly handle oat husks as an agricultural residue. However, this is a simplification, since husks today are used as animal feed and energy. Thereby, if oat husks are extracted from these already existing systems for dissolving pulp purposes, it is reasonable to assume a replacement of some other type of raw material for these applications. How this will affect the environmental performance of these connected systems would be interesting to evaluate in an additional assessment, to investigate possible environmental burdens in other systems caused by the introduction of the oat pulping plant. This type of assessment would, thereby, investigate which is the most environmentally beneficial application of oat husks, rather than the potential of using oat husks for dissolving pulp purposes.

6

Conclusion

This thesis provides an indication of the technical, economic and environmental performance of the production of dissolving pulp from oat husks. Due to simplifications, especially regarding chemical recovery and linearly upscaling of their inputs, the economic and environmental performance are expected to have high potential to be improved. Thereby, further research is needed to ensure the performance of dissolving pulp from oat husks. However, the results presented in this thesis indicate relatively good performance of oat husks for production of dissolving pulp as well as feasibility in industry. The results indicated a climate impact of approximately 950-1200 kg CO_2-eq/ton dry pulp, excluding biogenic carbon, which is slightly higher than a common climate impact of wood based pulp of 200-1000 kg CO_2-eq/ton dry pulp, excluding biogenic carbon.

Based on these indications, oat husks can be concluded to be a possible alternative raw material for the production of dissolving pulp, but for it to become a favorable alternative to wood, further development and optimisation of the pulping process, as well as its chemical inputs, are required.

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A

Appendix 1

A.1 Data provided from lab trials

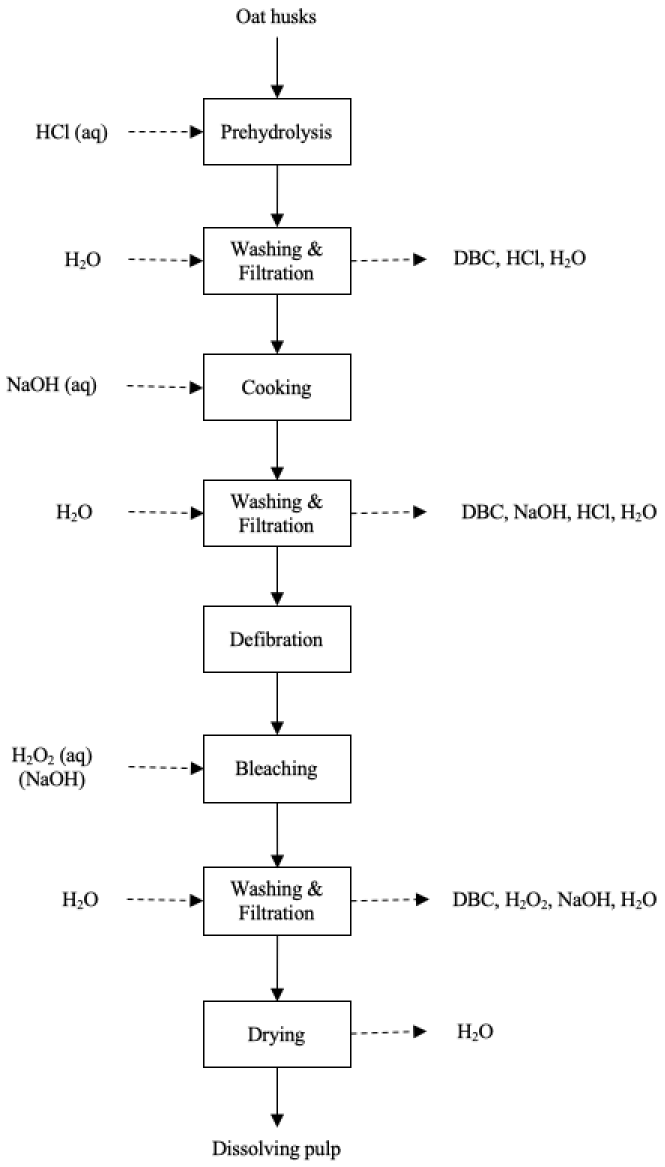

Figure A.1: Flow chart of lab pulping process from oat husks to dissolving pulp with all inputs and outputs, where DBC is abbreviation for dissolved biomass components. Derived based on provided information of lab trial.

Table A.1: Lab data of the composition of oat husks with a dry content of 90.3%

Component	wt%
Glucose	29.69
Xylan	29.74
Galactan	1.28
Arabinan	3.34
Lignin	22.22
ASL	2.61
Ash	5.85

A.2 Data for implementation in technical assessment

Table A.2: Total harvest of oats in different counties 2020 [1].

County	Oat harvest in 2020 [tonnes]
Västra Götaland	302 000
Halland	37 700
Skåne	75 500
Kalmar	7 700
Kronoberg	8 400
Jönköping	12 000
Östergötland	41 500
Total	484 800

Table A.3: User specified properties of biomass components in Aspen Plus. Where NATOM descibres the chemical formula, DHSFRM the solids heat of formation at 25ºC, VSPOLY the molar volume parameters of solid, CPSPO1 the solid heat capacity coefficients and MW the molecular weight [2].

Component	NATOM	DHSFRM [cal/mol]	VSPOLY [cum/kmol]	CPSPO1 [kJ/kmol-K]	MW [g/mol]
Cellulose	$C_6H_{10}O_5$	-233200	$C_1 = 0.249$	$C_1 = -1.5328$; $C_2 = 0.67527$	
Galactan	$C_6H_{10}O_5$	-233200	$C_1 = 0.249$	$C_1 = -1.5328$; $C_2 = 0.67527$	
Mannan	$C_6H_{10}O_5$	-233200	$C_1 = 0.249$	$C_1 = -1.5328$; $C_2 = 0.67527$	
Xylan	$C_5H_8O_4$	-182100	$C_1 = 0.203$	$C_1 = -1.2489$; $C_2 = 0.55022$	132.117
Arabinan	$C_5H_8O_4$	-182100	$C_1 = 0.203$	$C_1 = -1.2489$; $C_2 = 0.55022$	132.117
Lignin		-108248		$C_1 = -0.472915$; $C_2 = 0.79267$	

A.3 Specification of settings in Aspen Plus

Table A.4: Process units in Aspen Plus model, specified in regard to name, type, process step, purpose and what unit they simulate in industry. The numbers of units required in industry are specified within parenthesis under "Industry unit".

Name	Type	Process step	Aim	Industry unit (nr)
MIX1	Mixer	Prehydrolysis	Enter inputs	Digester (4)
PUMP1	Pump	Prehydrolysis	Increase P	Pump
HEAT1	Heater/HX	Prehydrolysis	Increase T	Digester (4)
PREHYD	RSToic reactor	Prehydrolysis	Prehydrolysis	Digester (4)
SEP1	Separator	Prehydrolysis	Filter BL	Digester (4)/Filter
MIX2	Mixer	Cooking	Enter inputs	Digester (4)
PUMP2	Pump	Cooking	Increase P	Pump
HEAT2	Heater/HX	Cooking	Increase T	Digester (4)
COOK	RSToic reactor	Cooking	Cooking	Digester (4)
SEP2	Separator	Cooking	Filter BL	Filter
WASH1	SWash	Washing 1	Wash pulp	Washing
WPUMP1	Pump	Washing 1	Pump washing water	Washing
SEP3	Separater	Washing 1	Filter in WASH1	Filter
MIX3	Mixer	Bleaching	Enter inputs	Bleaching stages (3)
HEAT3	Heater/HX	Bleaching	Increase T	Bleaching stages (3)
BLEACH	RSToic ractor	Bleaching	Bleaching	Bleaching stages (3)
SEP4	Component separator	Bleaching	Filter & DSB	Filter
WASH2	SWash	Washing 2	Wash bleached pulp	Washing
WPUMP2	Pump	Washing 2	Pump washing water	Washing
SEP5-DRY	Separator	Dryer	Filter & drying	Filter/drier

Table A.5: Prehydrolysis process flows in Aspen Plus model, specified in regard to name, flow content, temperature (T) and pressure (P).

Name	Flow of	T [°C] : P [bar]
OATHUSKS	Oat husks	25 : 1
PRELIQ	Prehydrolysis liquor	25 : 1
PREIN	OATHUSKS in PRELIQ	25 : 1
PREINP	PREIN with increased P	25 : 7
PREINH	PREINP with increased T	160 : 7
PREOUT	Prehydrolysed mass & liquor	160 : 7
BL1	Black liquor	160 : 7
PREDONE	Prehydrolysed mass	160 : 7

Table A.6: Cooking process flows in Aspen Plus model, specified in regard to name, flow content, temperature (T) and pressure (P).

Name	Flow of	T [°C] : P [bar]
COOKLIQ	WL	25 : 1
COOKIN	PREDONE in COOKLIQ	83 : 1
COOKINP	COOKIN with increased P	83 : 8
COOKINH	COOKINP with increased T	170 : 8
COOKOUT	Pulp & liquor	170 : 8
BL2	Black liquor	170 : 8
COOKSEP	Pulp & liquor	170 : 8
WASHIN1	Washing water	25 : 1
WASHINP1	WASHIN1 with increased P	25 : 9
WASTE1	Residues of chemicals & water	103 : 2
COOKWASH	Washed pulp	103 : 2
WASTE 2	Residues of DSB, chemicals & water	103 : 2
COOKDONE	Washed & filtered pulp	103 : 2

Table A.7: Bleaching process flows in Aspen Plus model, specified in regard to name, flow content, temperature (T) and pressure (P).

Name	Flow of	T [°C] : P [bar]
BLELIQ	Bleaching liquor	25 : 1
BLEIN	COOKDONE in BLELIQ	71 : 1
BLEINH	BLEIN with increased T	80 : 1
BLEOUT	Bleached pulp & liquor	80 : 1
WASTE3	Residues of DSB, chemicals & water	80 : 1
BLESEP	Bleached pulp & liquor	80 : 1
WASHIN3	Washing water	25 : 1
WASHINP3	WASHIN3 with increased P	25 : 7
WASTE 4	Residues of chemicals & water	53 : 1
BLEWASH	Washed bleached pulp	53 : 1
SEPOUT6	Residuces of DSB, chemicals & water	53 : 1
DISSMASS	Dissolving pulp	53 : 1

Table A.8: Settings in process unit SEP1 for outlet stream PREDONE (Mixed) in Aspen Plus.

Component	Specification	Value	Units
Cellulose	Split fraction	0.15	
Xylan	Split fraction	0.15	
Arabinan	Split fraction	0.15	
Lignin	Split fraction	0.15	
ASL	Mass flow	307.245	kg/h
Ash	Split fraction	0.15	
Others	Split fraction	0.15	
Water	Mass flow	32161.5	kg/h
Hydrochloric acid	Split fraction	0.15	

Table A.9: Settings in process unit SEP2 for outlet stream COOKSEP (Mixed) in Aspen Plus.

Component	Specification	Value	Units
Cellulose	Split fraction	0.15	
Xylan	Split fraction	0.15	
Arabinan	Split fraction	0.15	
Lignin	Split fraction	0.15	
ASL	Mass flow	68.8363	kg/h
Ash	Split fraction	0.15	
Others	Split fraction	0.15	
Water	Split fraction	0.4	
Hydrochloric acid	Split fraction	1	
Sodium hydroxide	Split fraction	0.15	

Table A.10: Settings in process unit SEP3 for outlet stream COOKDONE (Mixed)in Aspen Plus.

Component	Specification	Value	Units
Cellulose	Split fraction	0.15	
Xylan	Split fraction	0.15	
Arabinan	Split fraction	0.15	
Lignin	Split fraction	0.15	
ASL	Mass flow	29.9039	kg/h
Ash	Split fraction	0.15	
Others	Split fraction	0.15	
Water	Mass flow	28016.6	kg/h

Table A.11: Settings in process unit SEP4 for outlet stream BLESEP (Mixed)in Aspen Plus.

Component	Specification	Value	Units
Cellulose	Split fraction	0.15	
Xylan	Split fraction	0.15	
Arabinan	Split fraction	0.15	
Lignin	Split fraction	0.15	
ASL	Split fraction	1	
Ash	Split fraction	0.15	
Others	Split fraction	0.15	
Water	Mass flow	28016.6	kg/h
Sodium hydroxide	Split fraction	0.15	
Hydrogen peroxide	Split fraction	0.15	

Table A.12: Settings in process unit SEP5-DRY for outlet stream DISSMASS (Mixed)in Aspen Plus.

Component	Specification	Value	Units
Cellulose	Split fraction	0	
Xylan	Split fraction	0	
Arabinan	Split fraction	0	
Lignin	Split fraction	0	
ASL	Split fraction	1	
Ash	Split fraction	0	
Others	Split fraction	0	
Water	Mass flow	4902.28	kg/h

Table A.13: Settings in process unit WASH1 & WASH2 in Aspen Plus.

Specifications	WASH1	WASH2
Liquid-to-solid mass ratio	5.8	5.75
Mixing efficiency	0.9	0.9
Pressure [bar]	2	No specification

Table A.14: Hourly input of the two alternative prehydrolysis liquors.

Liquor components	Inflow [kg/h]
Hydrochloric acid	93.81
Water	92035.51
Sulphuric acid	126.05
Water	92003.27

Table A.15: Hourly input of white liquor.

Liquor components	Inflow [kg/h]
Sodium hydroxide	3559.20
Water	53259.39

Table A.16: Hourly input of bleaching liquor.

Liquor components	Inflow [kg/h]
Hydrogen peroxide	2472.05
Sodium hydroxide	19.78
Water	18932.63

A.4 Additional results from simulation in Aspen Plus

Table A.17: Hourly outflow of dissolving pulp in industrial scale.

Dissolving pulp content	[kg/h]
Total	9804.6
Liquid	4902.3
Cellulose	4642.0
Galactan	0
Mannan	28.9
Xylose	193.2
Arabinan	2.9
Lignin	9.8
ASL	29.9
Ash	0
"Others"	0

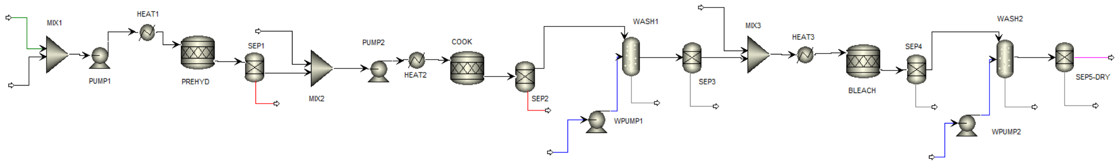

Figure A.2: Model of oat pulping process in Aspen Plus. Name of units specified above or below, name of flows in rectangles, temperatures (°C) in circles and pressures (bar) in hexagons.

A.5 Data for implementation in economic assessment

Table A.18: Estimated capital costs for a single process unit.

Unit	MSEK
Stepwise batch digester	100
Bleaching stage	80
Washing equipment	50
Screening equipment	30
Pump	0.075

The operating costs presented in Table A.19 are collected and estimated based on different references. The cost of oat husks is estimated based on the cost of forest residues for fuel production presented in *Tillgång på skogsråvara- sammanfattning och scenarier, en förstudie* by Sandin, T. S. Zetterberg, and T. Rydberg, 2019 as well as IVL estimation of its energy content. The cost of process water is estimated based on recommendations in *Chemical Engineering Design* by R. K. Sinnott and G. Towler, 2013.

Table A.19: Data used for operational costs.

Input	Value	Unit
Oat husks	160	SEK/MWh
Oat husks	0.02	MWh/kg
Sodium hydroxide	13346.68	SEK/ton [31]
Sulphuric acid	635.468	SEK/ton [31]
Hydrogen peroxide	3973.544	SEK/ton [31]
Process water	23	SEK/m^3
Electricity	0.27688	SEK/kWh [32]

Table A.20: Assumptions used for operational costs based on recommendations in *Chemical Engineering Design* by R. K. Sinnott and G. Towler, 2013 .

Parameter	Assumption
Allowance factor	1.45
Wages	35000 SEK/month
Workers	15
Supervision	20% of wages
Management	50% of wages
Maintenance	5% of CAPEX
Insurance	1% of CAPEX
Taxes	2% of CAPEX
Yearly cost increase	2%
Yeary increase in profit	2%

B

Appendix 2

B.1 Specification of settings in GaBi

Table B.1: Inflows into "Pulping process" in GaBi.

Inflow	Database setting
Oat husks	Project specific flow
Sodium hydroxide	EU-28: sodium hydroxide (caustic soda) mix (100%)
Sulphuric acid	EU-28: Sulphuric acid (96%)
Hydrogen peroxide	DE: Hydrogen peroxide (100% H2O2) (integrated prod., 70% H2 chemical synthesis, 40% raw solut.)
Elecitricty	SE: Elecitricty grid mix (production mix)
Water for liquids	EU-28: Tap water from surface water
Washing water	EU-28: Process water from surface water

Table B.2: Transportation of oat husks in GaBi.

Database setting	Diesel MK1 (Red-diesel 2022: 36.3% bio fuel (6% RME and 30.3% HVO))
Vehicle	Truck, 28-32 tot weight, MPL 22 t
Distance [km]	200
Load factor	0.85
Fuel sulphur content [ppm]	4

Table B.3: Transportation of sodium hydroxide, sulphuric aicd and hydrogen peroxide in GaBi.

Database setting	6% RME
Vehicle	Truck, 28-32 tot weight, MPL 22 t
Distance [km]	1500
Load factor	0.85
Fuel sulphur content [ppm]	6

B.2 Data for implementation in environmental assessment

Table B.4: Emissions from fuel production from forest residues, used as estimation of emissions from steam production in the recovery boiler [3].

Emission	[g/MJ]
Carbon dioxide	1.9
Methane	0.00014
Nitrogen oxides	0.012
Nitrous oxide	0.000064
Sulphur dioxide	0.00042

Table B.5: Global reference values for GWP (fos), AP, EP POF and ADP. Provided from IVL database.

Parameter	Global reference value	Unit
GWP (fos)	4.22E+13	kg CO_2-eq.
AP	2.40E+11	kg SO_2 eq.
EP	1.58E+11	kg Phosphate eq.
POF	3.45E+11	kg NMVOC eq.
ADP	3.61E+08	kg Sb eq.

B.3 Assessed impact categories in environmental assessment

Table B.6: All impact categories parameters, their assessment method and unit.

Impact category	Method	Unit
GWP (fos)	CML2001	kg CO_2 eq.
GWP (lnd)	CML2001	kg CO_2 eq.
GWP (tot)	CML2001	kg CO_2 eq.
AP	CML2001	kg SO_2 eq.
EP	CML2001	kg Phosphate eq.
POF	ReCiPe Midpoint (H)	kg NMVOC eq.
ADP	CML2001	kg Sb eq.
PERT	EN15804+A1	MJ
PENRT	EN15804+A1	MJ
FW	EN15804+A1	m^3
HDW	EN15804+A1	kg
NHWD	EN15804+A1	kg
RWD	EN15804+A1	kg

B.4 Specification of allocation method

Table B.7: Mass allocation of burden from sodium hydroxide and sulphuric acid on oat pulping plant (OP) and kraft mill (KM), determined based on the input of chemicals in the oat pulping plant and the amount of chemicals lost.

Chemical	In kg/ton pulp50	Lost kg/ton pulp50	Burden OP	Burden KM
Sodium hydroxide	367.44	118.89	66.2%	33.8%
Sulphuric acid	12.94	1.94	57.5%	42.5%

B.4.1 Mass allocation calculation

Allocated burden to the oat pulping plant (OP):

$$\text{Burden OP} = \frac{\text{Lost [kg/ton pulp50]} + \left(\frac{\text{(In [kg/ton pulp50]} - \text{Lost [kg/ton pulp50])}}{2}\right)}{\text{Input [kg/ton pulp50]}} \tag{B.1}$$

Allocated burden to the kraft mill (KM):

$$\text{Burden KM} = \frac{\text{(In [kg/ton pulp50]} - \text{Lost [kg/ton pulp50])}}{2 \cdot \text{In [kg/ton pulp50]}} \tag{B.2}$$

B.4.2 Specification of allocation method in sensitivity analysis

Table B.8: Mass allocation in sensitivity analysis of burden from sodium hydroxide and sulphuric acid on oat pulping plant (OP) and kraft mill (KM), determined based on the input of chemicals in the oat pulping plant and the amount of chemicals lost.

Chemical	In kg/ton pulp50	Lost kg/ton pulp50	Burden OP	Burden KM
Sodium hydroxide	367.44	118.89	32.4%	67.6%
Sulphuric acid	12.94	1.94	15.0%	85.0%

B.4.2.1 Mass allocation calculation

Allocated burden to the oat pulping plant (OP):

$$\text{Burden OP} = \frac{\text{Lost [kg/ton pulp50]}}{\text{Input [kg/ton pulp50]}} \tag{B.3}$$

B.5 Additional results from environmental assessment

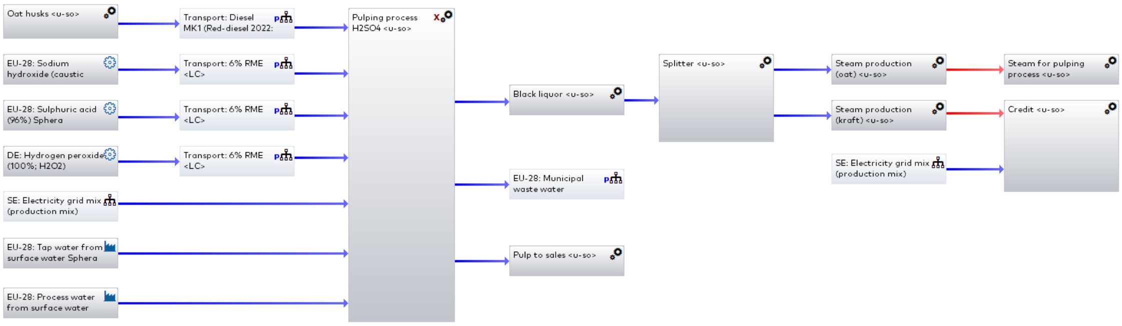

Figure B.1: Model of the assessed system in GaBi.

Table B.9: List of processes contributing to the environmental impact of the system and their abbreviations/names used in presentation of the results.

Process	Name in graphs
Waste water treatment	WWT
Transportation of hydrogen peroxide	Transp. H2O2
Production of sodium hydroxide	NaOH
Electricity production	El
Transportation of oat husks	Transp. oat husks
Production of sulphuric acid	H2SO4
Transportation of sodium hydroxide	Transp. NaOH
Production of hydrogen peroxide	H2O2
Water for liquids	Liq water
Transportation of sulphuric acid	Transp. H2SO4
Washing water	Wash water
Steam production	Steam production

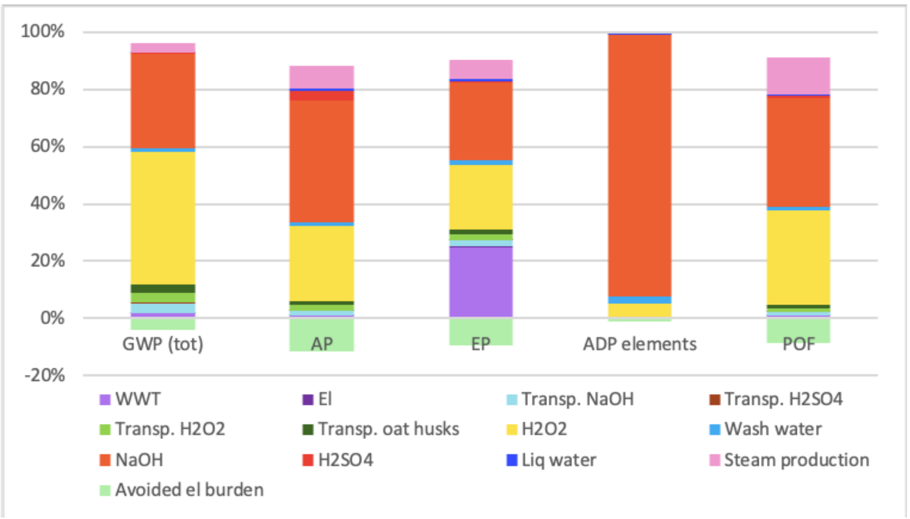

Figure B.2: Case B (avoid. el.) - percentile distribution of the burden in all processes for GWP (tot), AP, EP, ADP and PDF.

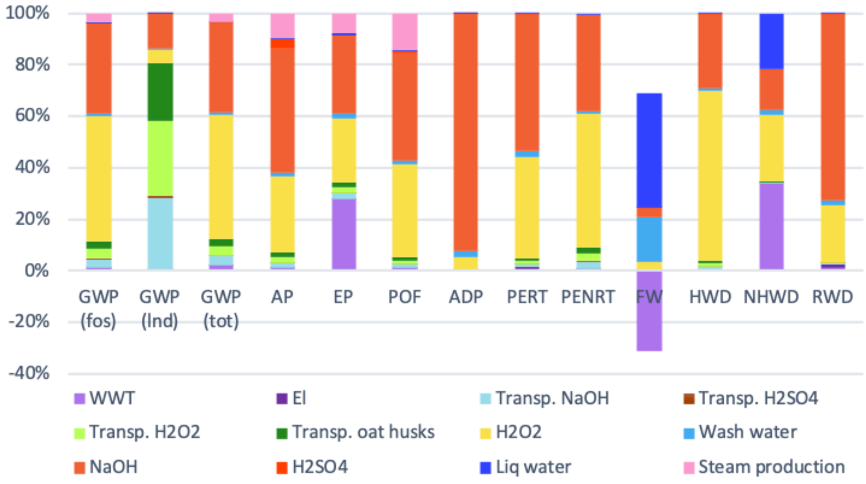

Figure B.3: Case A (no credit) - percentile distribution of the burden in all processes and all assessed impact categories.

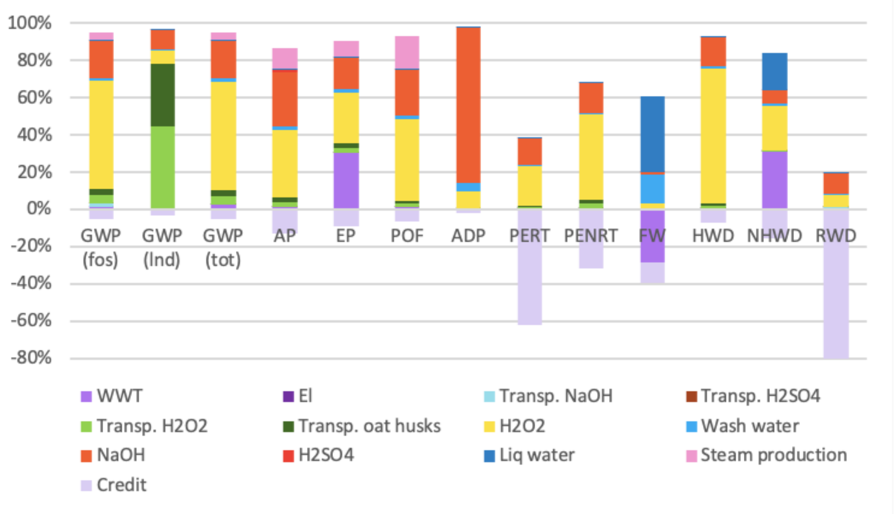

Figure B.4: Case D (SA credit) - percentile distribution of the burden in all processes and all assessed impact categories.

DEPARTMENT OF CHEMISTRY AND CHEMICAL ENGINEERING
CHALMERS UNIVERSITY OF TECHNOLOGY
Gothenburg, Sweden
www.chalmers.se

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