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Techno-economic and sustainability assessment

Circular cellulose to textile fiber production

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Preface

This document reports the findings from the techno-economic and sustainability assessment done in the project Circular cellulose to textile fiber production. The aim of the project has been to develop resource efficient processes for alternative cellulose feedstocks from residual streams to increase value for dissolving pulp, for e.g., textile fiber production. In this report, a techno-economic feasibility study and an environmental impact assessment were done to give an indication of the market relevance and climate impact of wheat straw and oat husk as raw materials for the production of dissolving pulp.

Summary

In this report, a techno-economic feasibility study and an environmental impact assessment were made in order to compare the production of dissolving pulp from wheat straw and oat husk and give an indication on the market relevance and climate impact of the processes.

The assessments done in this report are based on results of previous work done in the *Circular cellulose to textile fiber production* project. Previous works include experimentally evaluating and optimizing chemical routes of the production of dissolving pulp from agricultural residue as well as process simulations built on the experimental results and techno-economic and environmental impact assessments of the processes. In current report, the previous work has been complimented with additional simulations and evaluations required to obtain sufficient data to compare the technical, economic, and environmental performance of the two processes.

The process simulations and heat integrations were done in Aspen PLUS and Aspen Energy Analyzer and the environmental impact assessment was performed in the Life Cycle Assessment tool LCA for experts (formerly GaBi). Resource and energy demand, major equipment cost and minimum selling price of dissolving pulp, as well as 7 environmental impact categories and 2 resource indicators were studied. Furthermore, sensitivity analyses were performed on the economic and environmental impact results.

The results show that the wheat straw-based case have a better technical, economic, and environmental performance than the oat husk-based case. This is largely due to the fact that the wheat straw-based process has a higher yield (45%) than the oat husk case (31%). The yield affects the equipment size and cost, which in turn affects the total fixed capital investment (TFCI). The sensitivity analysis done on the results of the techno-economic assessment showed that TFCI was the parameter with the greatest impact on the minimum selling price of dissolving pulp (DP). Additionally, it was found that the largest contributor to the final price of dissolving pulp were chemicals and utility, followed by indirect costs and the cost of feedstock. The resulting minimum selling price for wheat straw and oat husk were 12.5 and 14.7 SEK/kg DP (compare to 10 SEK/kg DP indicated by industry).

The results of the environmental impact assessment showed that the cultivation of the feedstock has a significant impact on the environmental performance. As a

result, the case with the higher yield (wheat straw) exhibited lower climate change impact (1700 kg CO_2 eq./ ton DP) than the oat husk case (1820 kg CO_2 eq/ton DP). Moreover, it was found that steam produced from natural gas is the highest contributor to climate change impact for both cases. Changing the source of steam from natural gas to biomass reduces the climate change impact by 65% for both wheat straw- and oat husk-based pulp.

Based on the result of this report, it is recommended to focus on finding more optimized chemical routes for the production of dissolving pulp from agricultural residue. It is also of importance to find more optimized process and heat integration designs to make the processes less resource and energy intensive. This would result in an increased technical, economic, and environmental performance for both cases.

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1 Introduction

The global apparel industry is accountable for 6.7% of the global climate impact. The main impact stems from the fossil origin of the textile feedstock as well as the production processes (1). Man-made cellulosic fibers (MMCF) are an important alternative to fossil-based textiles and contributes to the conversion into a biobased and circular society. The major commercially available technology for production of MMCF is the viscose process, which is made from wood-based dissolving pulp (DP) but has drawbacks—high usage of the volatile and toxic chemical CS2, and a comparably high climate impact. On a total, MMCF only stands for 6.4% of the 111 million metric tons of global textile fiber produced in 2019 (2) why the development of new processes is the key to meet the increasing market demands, but even more importantly to accelerate the conversion from a fossil to a biobased society.

The TreeToTextile (TTT) process is designed to make a significant contribution to the biobased society as it converts wood-based dissolving pulp into a textile staple fiber using a sustainable and cost-efficient technology. The process depends on the properties of the extracted cellulose fraction, which opens up for the use of other cellulose rich biobased feedstocks.

This project (Circular cellulose to textile fiber production) will, in collaboration with TreeToTextile, Chalmers University of Technology and Stora Enso, develop resource efficient processes for alternative cellulose feedstocks from residual streams to increase value for dissolving pulp, for e.g., in textile fiber production. The cellulose rich resources to be processed is agricultural waste streams (e.g., oat husk), recycled carton board/paper, and recycled textiles (i.e., cotton and viscose), which will be available in bulk and converted into dissolving pulp as a substitute for wood-based dissolving pulp. The purpose is to enable a circular cellulose economy in Sweden, as part of a circular bioeconomy. By increasing the resource efficiency in the alternative raw material flows such as dissolving pulps can be found attractive in for example regenerated man-made cellulosics, which will be validated by the textile fiber process available at TreeToTextile.

The research will develop processes to produce tailored dissolving pulps from biobased residues and generated knowledge on their properties and how these may be controlled. Such information together with the techno-economic feasibility and sustainability performance will generate value, also by other stakeholders within the cellulose industry to support in their strategies and efforts towards increased innovation in the transition to a circular bioeconomy.

1.1 Aim

In this report, a techno-economic feasibility study and an environmental impact assessment will be made in order to give an indication on the market relevance and climate impact of different feedstocks and usages. The techno-economic and environmental assessments will be based on results from previous work packages (WPs) where a selection of 4 cellulosic waste streams were selected (WP1) and a resource efficient chemically feasible route were optimized for each waste stream (WP2).

1.2 Summary of previous work

Previous work done in this project aimed at collecting data (i.e., volumes, availability, etc.) for a couple of different cellulosic residue streams. From the data collected, 4 different residue streams were selected to be processed to find a route for conversion of the streams into dissolving pulp. The 4 residue streams selected were oat husk, wheat straw, pressed sugar beet, and potato pulp.

The 4 cellulosic residues were investigated to find optimized extraction and separation process routes for each residue stream. Processes investigated included refining, pre-hydrolyzed kraft pulping (PHK), bleaching or just hydrolysis pretreatment to adjust the chain length of the cellulose. Cellulose properties analyzed were the yield, carbohydrates (purity), molecular chain length, molecular weight distribution together with chemical demand and estimated energy usage. Following the optimization and analysis of different extraction and separation routes, potato pulp and pressed sugar beet were excluded from further study.

The chosen 2 residue streams were oat husk and wheat straw. These raw materials were chosen because of their abundance in Sweden, their low lignin content and relatively high cellulose content. The process chosen was the pre-hydrolysis-soda pulping process, where a pre-hydrolysis step is used to remove hemicelluloses and facilitate delignification, and soda pulping is used as the main delignifying step (3). An acid pre-hydrolysis-soda pulping process followed by a total chlorine-free (TCF) bleaching sequence was proven to be suitable for oat husk. The produced pulps had uniform molecular weights, high cellulose content, low hemicellulose content and little to no lignin content. The acid pre-hydrolysis was efficient in removing hemicelluloses and facilitated delignification in the soda pulping step. With a higher liquid to solid ratio in the acid pretreatment and higher concentrations of NaOH during cooking, wheat straw exhibited similar properties regarding molecular weight distribution, cellulose, and hemicellulose contents.

The details of the experiments and optimization of the chemical routes of producing dissolving pulp from wheat straw and oat husk can be found in the work done by Sjöstedt (3). The scale-up of the optimized chemical routes were done using the modelling software Aspen Plus and the heat integration for the two cases was done using Aspen Energy Analyzer. The details and assumptions, as well as the model set-ups and simulation results for the oat husk and wheat straw case can be found in the works done by Ulefors (4) and Nilsson (5) respectively.

Following the scale-up and simulations a techno-economic assessment and an environmental impact assessment were performed to evaluate the feasibility of using wheat straw and oat husk as feedstock for production of dissolving pulp. The environmental impact assessment was done using the Life Cycle Assessment tool LCA for experts (formerly GaBi). The details of the evaluations of oat husk and wheat straw can be found in the works done by Ulefors (4) and Parayil (6) respectively.

Presented in this report will be the results of the process simulations of dissolving pulp production from wheat straw and oat husk, as well as the techno-economic assessment and environmental impact assessment based on the simulation results.

1.3 Theory

In the following section an overview of the feedstock composition, dissolving pulp characteristics and a brief description of the pulping process will be presented. Furthermore, information about the life-cycle assessment (LCA) methodology used in this work is presented at the end of the section.

1.3.1 Feedstock composition

Lignocellulosic biomass is the most abundant renewable feedstock. Lignocellulosic biomass can be classified either as non-wood or wood. Non-wood lignocellulosic consists of biomass derived from plant-based sources such as agricultural residues and other plant fibers, for example cotton and sugarcane (7). The cell wall of lignocellulosic biomass consists of cellulose, hemicellulose, lignin, and extractives (5). The distribution of these components varies between different types of biomasses but has in common that the main component is cellulose (33-51%), followed by hemicellulos (19-34%) and lignin (20-30%) (8). In recent years, lignocellulosic biomass has gained interest as a renewable resource for biomaterials since it has a wide availability and can be cost-effective when it comes to processing (7).

1.3.1.1 Wheat straw

Wheat straw is a byproduct from wheat farming that is used today as animal feed, fertilizer, fuel and to a small extent, as a base material in pulp production (5). Wheat straw consists of roughly 34-40% cellulose, 20-25% hemicelluloses and 20-25% lignin (9). In Europe at least one third of the wheat straw is required to remain on the field in order to ensure that a sufficient amount of nutrients is kept in the field. Around 20% of wheat straw is needed for bedding and animal feed. The rest of the wheat straw can be utilized for energy and other production areas. There is potential to increase the use of wheat straw for energy and other production areas as there is more straw available than what is being used. The amount of straw acquired from harvesting wheat varies between 0.5-1.4 straw/grain ratio.

1.3.1.2 Oat husk

Oat husks comprise approximately 30% of the oat weight and differs from wood not only in form and size but also in composition (4). It consists of 15-25% cellulose, 20-35% hemicelluloses, and 10-30% lignin (10). Oat husks, thereby, have a lower content of cellulose than wood, which usually have a cellulose content above 40%. Today, oat husks are mainly used as raw material for energy production and as animal feed.

1.3.2 Dissolving pulp

Dissolving pulps are a starting material for the production of cellulose derivatives and textile fibers (7). There are different processes for producing textiles from dissolving pulp, such as the viscose and lyocell process. The dissolving pulp requires a cellulose content of more than 90% and a hemicellulose content of less than 6%. The dissolving pulp should also only contain trace amounts of lignin and other impurities.

The intrinsic viscosity is another important property of dissolving pulp (7). It is a measurement of the size of the polymer in the solution and hence proportional to the molecular weight. If it is too low, it can cause a gel-like swelling and make filtration difficult. A low intrinsic viscosity also indicates a low physical strength of the pulp. However, if it is too high it can cause inhomogeneity. Usually, a viscosity of between 400 – 600 mL/g is desired, which is then reduced to 200 – 250 mL/g during the textile making process.

A high cellulose reactivity is another important property (7). This means that the cellulose has a high capacity to partake in diverse chemical reactions. If the reactivity is too low, it can cause problems during the textile making process such as plugging of spinning nozzles or decreased product yield. A high accessibility and reactivity can be achieved if the dissolving pulp has a high porosity, large pore size and high surface area. The reactivity partially depends on the raw material, but can be improved by mechanical, chemical, or enzymatic treatment.

A uniform molecular weight distribution of the dissolving pulp is also desirable and ensures homogeneous reactions during the textile making process (7). Another property of interest is the ISO brightness. This is required to be between 89-93% for viscose fibers.

1.3.3 Soda cooking

In soda cooking, sodium hydroxide is used to delignify the biomass, the process also breaks down polysaccharides (5). The cooking can be performed either batchwise or continuously and is typically operated at temperatures between 150°C and 170°C. As it is not desired for the cooking liquor to vaporize, the cooking takes place in pressurized vessels called digesters. After cooking, the pulp is recovered and sent to further processing, where it is washed and bleached to reach desired properties. Black liquor, which consists of spent cooking liquor and dissolved biomass can be sent through a chemical recovery process which recovers the cooking liquor whilst also providing energy for the pulping process.

Soda cooking is considered to be a more environmentally friendly pulping technology compared to standard chemical pulping processes such as kraft pulping or sulfite pulping (5). This is because soda cooking uses fewer chemicals and does not produce toxic gases such as hydrogen sulfide or sulfur dioxide. The soda cooking also consumes less chemicals making it more suitable for raw materials with a lower lignin content and is in general used for non-wood materials.

1.3.3.1 Black liquor treatment

The chemical recovery of black liquor consists of five steps:

1. Black liquor evaporation in multiple-effect evaporators, where the weak black liquor is evaporated from around 15 wt-% dry solids (DS) to heavy black liquor with a DS of 65-85 wt-%.
2. Condensate treatment.
3. Combustion of the organic fraction of the black liquor in the recovery boiler to generate steam and produce a smelt, which are molten inorganic salts. The smelt is dissolved in water, creating what is referred to as green liquor.
4. Causticization of green liquor to white liquor by the addition of lime (CaO). This is done by adding water and CaO together with the green liquor in a slaker. Here the CaO is converted to $Ca(OH)_2$ and reacts with the Na_2CO_3 in the green liquor to form NaOH and $CaCO_3$ (lime mud).
5. Calcination/Lime-mud burning to generate the lime used for the causticization. The white liquor is passed through a white liquor clarifier to remove the lime mud. The lime mud is sent through the mud washer and is then dried and sent to the calcination process to recover the CaO. The calcination can either be done in a conventional lime kiln or through electric plasma calcination.

This process generates steam, recovers cooking chemicals, and provides the pulping process with wash water (5).

1.3.4 Life cycle assessment

In order to assess the environmental performance of the above-mentioned processes, a LCA was conducted. An LCA investigates the environmental impacts occurring throughout the whole life cycle of a product or system. This includes evaluating energy and resource consumption as well as emissions from all life cycle stages including material production, manufacturing, use and maintenance and end of life. However, in this study the use phase and end of life of dissolving pulp were not considered as these impacts will be independent of the process routes through which dissolving pulp is produced. This type of LCA, with such a system boundary is known as a cradle to gate LCA. There are four steps in an LCA as per the ISO 14040/14044 standards, which are –

1. Goal and Scope Definition
2. Life Cycle Inventory Analysis
3. Life Cycle Impact Assessment

4. Interpretation of Results

2 Methodology

In the following section the frameworks of the techno-economic and environmental assessment are presented. The section contains the setup of the process simulations in Aspen PLUS and Aspen Energy Analyzer performed to obtain the mass and energy flows used for the evaluation of the processes. Furthermore, the methods and parameters used for the economic and environmental analysis are presented.

2.1 Process simulations

In the present work the production of dissolving pulp from wheat straw and oat husk are simulated with the aim to obtain the mass and energy balances needed for a techno-economic assessment and an environmental impact assessment.

In order to derive mass and energy balances for the 2 scaled-up processes (wheat straw and oat husk) flowsheets of the processes were simulated in Aspen Plus. The plants are assumed to be located in Sweden, with an annual operational time of 8400h corresponding to 95.9% of the year. The scale-up of the experimental results was done based on a framework developed for scaling up chemical processes for life cycle assessment studies (11). The thermodynamic model electrolyte non-random two liquids (ELECNRTL) was applied to the wheat straw case and the non-random two liquids (NRTL) thermodynamic model was applied to the oat husk case. The production capacity was set to 45.1 and 45.4 kton of air-dried dissolving pulp per year for wheat straw and oat husk respectively. The process flow diagram of the two processes that were simulated in Aspen Plus is presented in Figure 1.

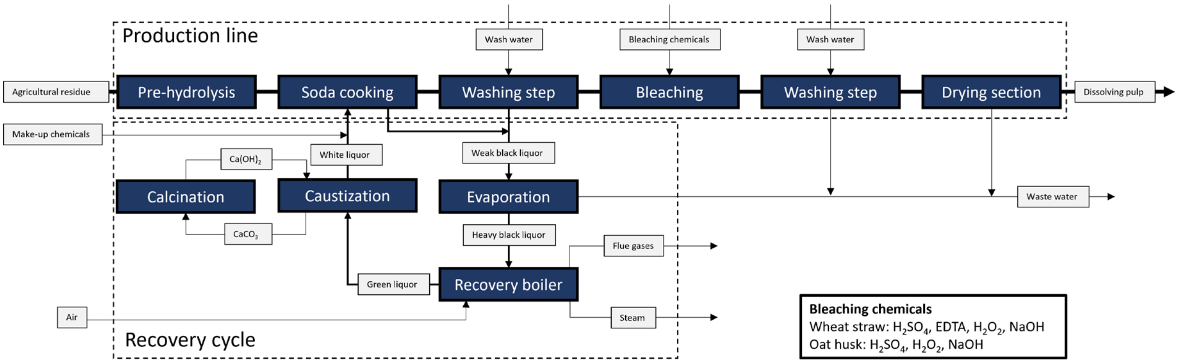

Figure 1. Process flow diagram of dissolving pulp production from agricultural residue.

The feedstock is first processed through pre-hydrolysis at 7 bar and 160°C and then sent to the digester where the biomass is cooked with white liquor at 8 bar and 170°C. The black liquor is sent to the recovery cycle, where an evaporator train consisting of 5 effects are used to increase the DS content from 15 wt-% to 85 wt-%. The heavy black liquor is sent to the recovery cycle in order to recover the pulping chemicals. The pulp is sent through washing and filtration and then sent to the bleaching step where H_2O_2 and NaOH are used in the oat husk process and H_2O_2, NaOH, EDTA and H_2SO_4 are used in the wheat straw process. After the bleaching step, the pulp is washed in a second wash stage and then sent to a mechanical press where the pulp is pressed to a moisture content of 50 wt-%. Finally, the pulp is dried from 50 wt-% to 10 wt-% in the dryer section.

For detailed information of the process simulation set-ups and results for the wheat straw and oat husk process, see the work done by Nilsson (5) and Ulefors (4) respectively.

The work done by Nilsson and Ulefors did not include the caustization and calcination plant. Therefore, in this work, a simulation of the caustization and calcination plant was performed in Aspen PLUS. The calcination plant was simulated as an electric plasma calcination instead of the conventional lime kiln. The sizing and cost calculations are presented in Appendix A. The resulting costs were integrated in the overall techno-economic and life cycle impact assessment of the two cases.

2.2 Economic analysis

The economic analysis was performed based on the costs of the major process units, which were sized based on mass and energy balances obtained from the Aspen Plus simulations and the heat integration done in Aspen Energy Analyzer.

The total fixed capital investment (TFCI) was calculated using the factorial method proposed by Towler and Sinnot (12). The major equipment cost is calculated using Equation (1),

$$C_e = a + b \cdot S^n \tag{1}$$

where C_e is the purchase equipment cost in U.S. Gulf Coast basis, a and b are cost constants and S is the size parameter and n is the exponent for the particular equipment. The total purchase equipment cost was thereafter multiplied by a factor derived from the factors presented in Table 1 to obtain the TFCI.

Table 1. Factors for Estimation of Project Fixed Capital Cost (12).

Major equipment, total purchase cost	PCE
f_{er} Equipment erection	0.50
f_p Piping	0.60
f_i Instrumentation and control	0.30
f_{el} Electrical	0.20
f_c Civil	0.30
f_s Structures and buildings	0.20
f_l Lagging and paint	0.10
PPC = PCE × ($1+f_{er}+f_i+f_{el}+f_c+f_s+f_l$)	3.20
Design and engineering (D&E)	0.25
Contingency (X)	0.10
Fixed capital cost factor = PPC × (1+D&E+X)	4.32

The process equipment costs (PEC) were updated to 2022 values using a chemical engineering plant cost index (CEPCI) of 813. The values reported refers to SEK value 2022. The working capital was calculated as 5% of the TFCI.

To calculate the production cost of dissolving pulp produced from wheat straw and oat husk respectively, fixed and variable operating costs were calculated from the data presented in Appendix B.

In order to determine if the production of dissolving pulp from the cellulose residue streams would be profitable, the minimum dissolving pulp selling price was evaluated for each case. Based on the work done by Mesfun et al. (13) the production of dissolving pulp was assumed to reach full scale production after three years, assuming that the first year has a production of 30% of full capacity and the second year had a production of 70% of full capacity. Total capital investment was spread out over three years, with 40% of the TFCI invested the first year, 50% the second year and the last 10% the third year. The minimum selling price was calculated using a discounted cash flow model, using a discount rate of 10% and an economic lifetime of the plant set to 10 years. The minimum selling price was calculated so that the Net Present Value (NPV) would be 0. The calculation of NPV is presented in Equation (2),

$$NPV = \sum_{t=0}^{n} \frac{R_t}{(1+i)^t} \tag{2}$$

where t is number of years, i is discount rate of return and R_t is cash flow at year t. The full calculations are presented in Appendix C.

The oat husk case did not include the chemical recovery cycle. However, in order to be able to compare the two cases and to give a reliable estimate of the costs, it is important to include it in both cases. Since the two cases have a similar recovery cycle, the equipment and energy need for the oat husk case were estimated based on the equipment size and energy demand of the wheat straw case. The estimation was done using Equation (3),

$$\frac{Cost_2}{Cost_1} = \left(\frac{Capacity_2}{Capacity_1}\right)^m \tag{3}$$

which correlates cost with capacity. The exponent m may vary, but the average is close to 0.6, why it is referred to the “six-tenths rule” (14). The estimated equipment and utilities, along with the estimated costs, are presented in Appendix D.

2.3 Environmental assessment

Goal and scope definition

The goal of the LCA was to investigate the environmental impacts of producing dissolving pulp from oat husk and wheat straw as feedstock via the soda cooking process. The scope of the study is a cradle to gate prospective attributional LCA in which the processing of all chemicals required, raw materials along with their transport up to the point where dissolving pulp leaves the gate of the industry is considered. All environmental impacts are expressed per unit of functional unit which for this system was defined to be 1 ton of dissolving pulp produced. A detailed description on the goal and scope can be found in Appendix E.

The LCA carried out, studied the following set of indicators and impact categories shown below in Table 2. The method of impact assessment chosen for most indicators was Environmental Footprint 3.0 as per the recommendation of the EU commission for LCA impacts regarding goods and services. In all other cases the Environmental Product Declaration (EPD) international system's methodological preference was chosen. A better understanding on the different indicators and justification regarding their choice can be found in (6).

Table 2. Impact categories and indicators studied in the LCA.

Impact Category / Indicator	Unit	Method
Climate Change (CC)	kg CO2 eq.	EF 3.0
Abiotic Depletion Potential, non-fossil resources (ADP)	kg Sb eq.	EN15804+A1
Eutrophication Potential (EP)	kg Phosphate eq.	CML 2001
Photochemical Oxidation formation (POF)	kg NMVOC eq.	ReCiPe 1.05 Midpoint (H)
Acidification Potential (AP)	Mole H+ eq.	EF 3.0
Ozone Depletion Potential (ODP)	kg CFC-11 eq.	EF 3.0
Water Deprivation	m^3 world eq.	EF 3.0
Total use of renewable primary energy (PERT)	MJ	EN15804+A1
Total use of non-renewable primary energy (PENRT)	MJ	EN15804+A1

Figure 2 below shows the different activities studied in the LCA for both wheat straw based and oat husk-based pulp. As can be observed from the flowchart, the various activities are split into a foreground and background system. The production of the different chemicals used, as well as the cultivation of crops have been included in the modelling of the LCA. The raw materials required to produce dissolving pulp were assumed to come from Skåne county. The transport of all raw materials was assumed to be by truck.

The energy required for plant operations were modelled with values from process simulation and heat integration. The values are updated from the works done by Ulefors (4) and Nilsson (5). A base case was defined for the study with the following considerations - the source of steam to be from natural gas, no recycling of wastewater within the plant and the feedstock entering the system with an allocated environmental burden.

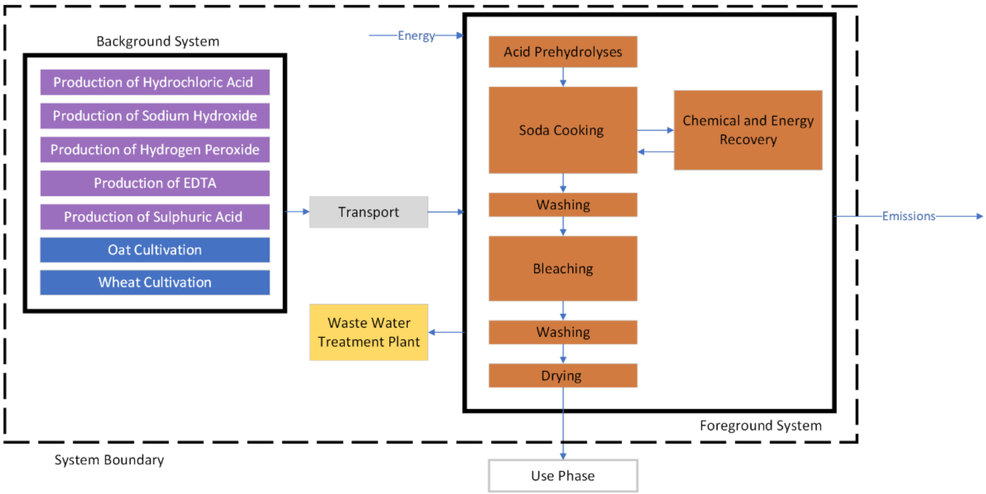

Figure 2. Flowchart showing the different activities studied in the LCA, for both oat husk and wheat straw-based pulp.

From the plant, emissions arise when black liquor is burnt to recover energy. The values for emission data were taken from the European Commission's Best Available Technology (BAT) guidelines for the paper and pulp industry (18). These emissions were assumed to remain the same irrespective of the raw material used and their values are found in Table 3. Emissions also arise in the calcination process within the lime kiln, but these are biogenic as the source is still biomass. The uptake and release of biogenic carbon is considered to be net zero over a long period of time. In a traditional plant the additional fuel used would cause emissions but for this system an electrical arc furnace was assumed to be used, thereby eliminating any use of fuel and further emissions arising from its burning.

Table 3 Emission values for pollutants from recovery boiler operations

Pollutant (emission to air)	**Amount (kg/ton dissolving pulp)**
Sulphur dioxide	0.002-0.65
Total Reduced Sulphur	0.0007-0.4
Nitrogen oxides	0.73-2.0
Particulates	0.02-1.6

Average emission values from Table 3 above were entered in the LCA model and simulated. For the LCA a generic wastewater treatment plant was also modelled, which would handle all the wastewater streams generated. This however is not part of the plant and is not modelled in the process simulation tool. The purpose of adding it in to the LCA was to study environmental performance of handling the amount of wastewater streams. Detailed explanations, choice of parameters and settings can be found in (6).

3 Results

The following section contains the results of the process simulations of the two cases, along with the results of the techno-economic assessment and the life cycle impact assessment of the studied systems. Furthermore, results of sensitivity analyses of the results of the techno-economic assessment and life cycle impact assessment are presented.

3.1 Process performance

The input and output streams of the wheat straw and oat husk processes are presented in Table 4.

Table 4. Feedstock, chemical usage, utility demand, emissions, product and yield of the production process of dissolving pulp from wheat straw and oat husk.

Feedstock	Unit	Wheat straw	Oat husk	Remark
Wheat straw	kg/h	11 905	-	11.4 wt-% moisture content
Oat husk	kg/h	-	17 314	9.7 wt-% moisture content
Chemicals				
Hydrochloric acid (HCl)	kg/h	175	-	
Sulfuric acid (H_2SO_4)	kg/h	15.7	13.4	
Sodium hydroxide (NaOH)	kg/h	196	171	Make-up chemicals (95% of NaOH assumed to be recovered)
Calcium oxide (CaO)	kg/h	56.8	71.5	Make-up chemicals
EDTA	kg/h	26	-	
Hydrogen peroxide (H2O2)	kg/h	456	215	
Utilities				
Process water	kg/h	96 670	572 712	
Steam	MW	21.7	21.6	8 bar steam used in evaporators 60 bar steam produced in recovery boiler
Electricity	MW	11.3	12.2	
Product				
Dissolving pulp	ADt/h	5.4	5.4	10% moisture content
Process				
Yield	%	45	31	ADt dissolving pulp/tonne feedstock

The feedstock are wheat straw and oat husk, with moisture content of 11.4 wt-% and 9.7 wt-% respectively. The product of the processes is dissolving pulp, dried to 10% moisture. The wheat straw process and the oat husk process needed 11.9 t/h and 17.3 t/h of feedstock respectively. The soda cooking process resulted in 5.38 Adt/h and 5.41 Adt/h of dissolving pulp for the wheat straw and oat husk case. The yield of dissolving pulp is about 45% and 31% for wheat straw and oat husk.

The amount of steam required for the processes are about 21 MW for both processes and the electricity demand are 11.3 MW for wheat straw and 12.2 MW for oat husk. The energy demand for different process steps can be seen in the work done by Ulefors (4) and Nilsson (5).

As can be noted, the wheat straw process required HCl and EDTA, which was not used in the oat husk process. Overall, the oat husk case requires less cooking and bleaching chemicals than the wheat straw process. This result aligns well with the experimental results reported by Sjöstedt (3).

It should be noted that the amount of process water in the oat husk process is almost 10 times the amount of the process water demand for the wheat straw process.

3.2 Economic performance

The major equipment costs for the scaled-up processes are presented in Figure 3. The major equipment account for approximately 175 MSEK and 201 MSEK of the total plant cost for wheat straw and oat husk respectively.

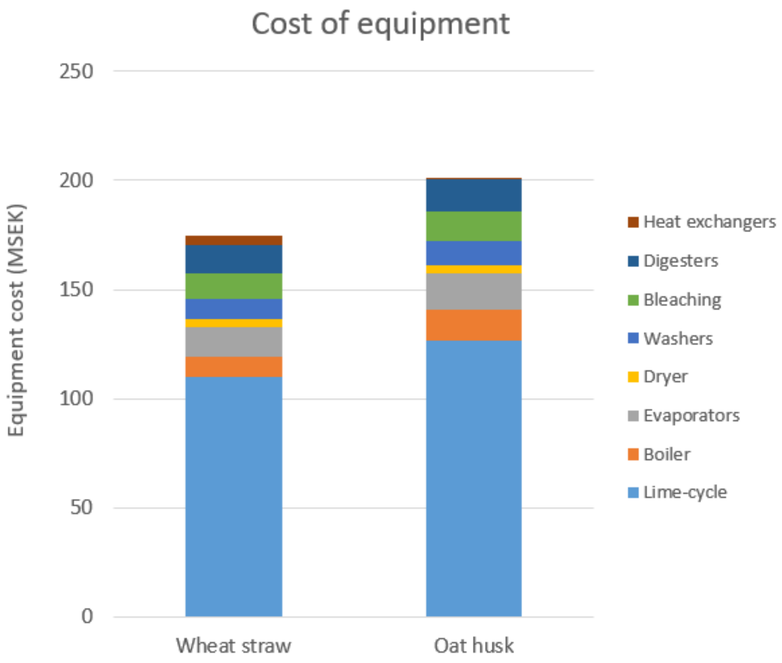

Figure 3. Cost of major equipment for production of dissolving pulp using wheat straw or oat husk as feedstock.

As can be seen, the largest contributor is the equipment associated with the lime-cycle, the following two largest contributors are the evaporators and the digesters. The feedstock and chemical costs per produced kg of dissolving pulp are presented in Figure 4.

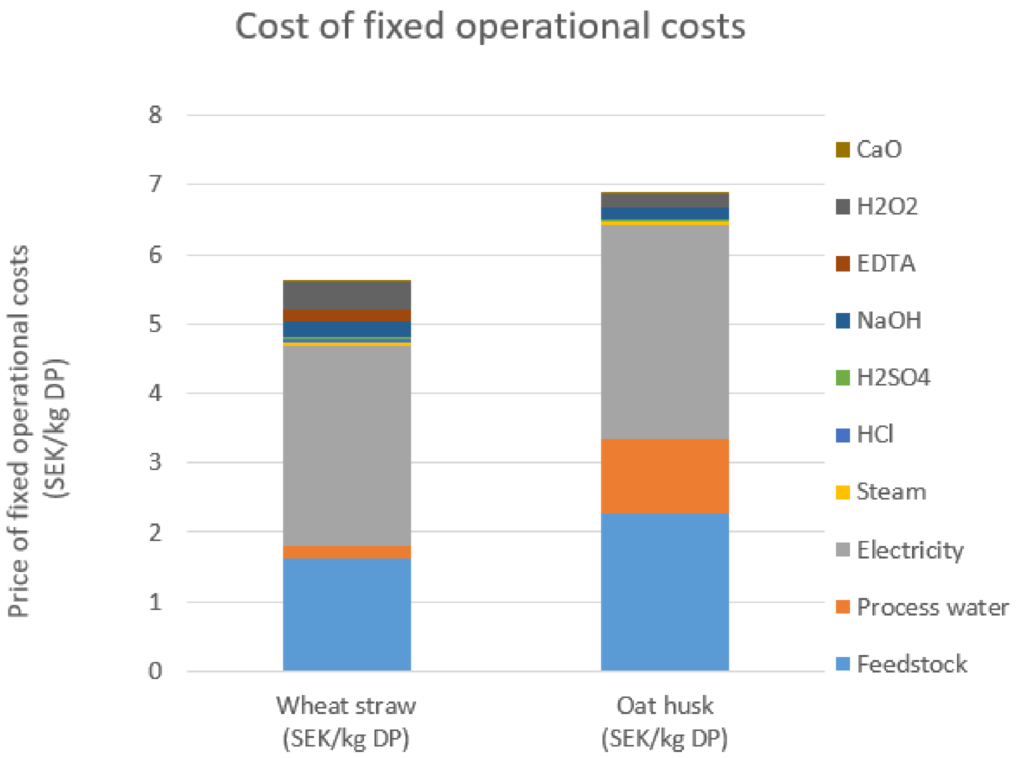

Figure 4. Fixed operational costs to produce dissolving pulp using wheat straw and oat husk as feedstock.

Worth noticing is that the main contributors to the operational cost is the feedstock and electricity. For the oat husk case, the process water is also a major contributor to the operational cost.

3.2.1 Production cost

The assessment was done based on the operational and capital costs as well as the parameters presented in Section 2.2 and Appendix B. The cost calculations are presented in Appendix C. The results of the economic analysis showed that both wheat straw and oat husk results in a minimum selling price of dissolving pulp above the price indicated by industry of 10 SEK/kg DP (4). The cost build-ups and minimum selling prices for dissolving pulp produced from wheat straw and oat husk that are required for a NPV of zero are presented in Figure 5.

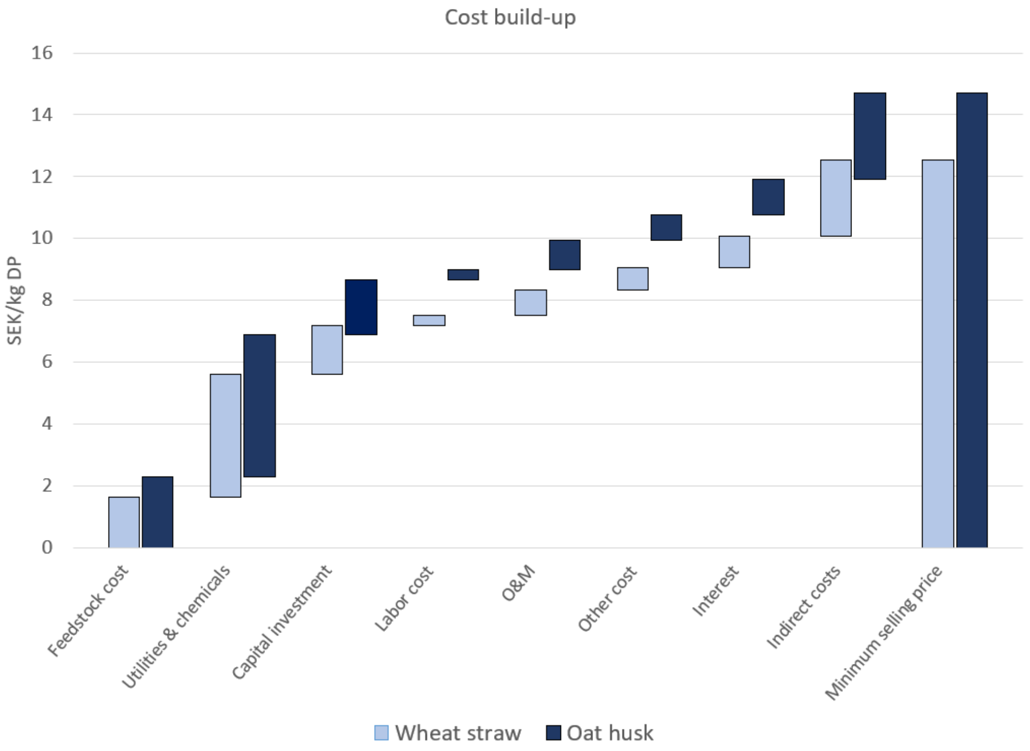

Figure 5. Cost build-up to minimum selling price for dissolving pulp production from wheat straw and oat husk.

The resulting minimum selling price are 12.5 and 14.7 SEK/kg DP for wheat straw and oat husk respectively. They main contributors to the cost build-up are the utilities and chemicals (31.9% and 31.3%), indirect costs (19.5% and 18.9), feedstock (12.9% and 15.5%), and cost of capital (12.5% and 12.2%).

The utilities and chemicals are the largest contributor to the cost build. The electricity required for drying of biomass is the main utility cost for both processes, while the major chemical cost constitutes of cost of sodium hydroxide and hydrogen peroxide. The major difference between wheat straw and oat husk in regard to the utility and chemical usage is the larger amount of process water required for the oat husk process.

The second largest contributor to the cost build-up is the indirect costs which included laboratory costs, plant overheads, capital charges, insurance, taxes, and royalties.

Feedstock cost is the third largest contributor. The price of oat husk (0.71 SEK/kg) is marginally lower than that of wheat straw (0.73 SEK/kg). However, since the yield of the wheat straw process is higher than that of oat husk, the cost of feedstock is higher for the oat husk process.

3.2.2 Sensitivity analysis

A sensitivity analysis was performed in order to account for the uncertainties of technical, economic and market factors. The technical uncertainties are related to the scale-up from laboratory scale to industrial scale and affects TFCI as well as chemical, utility, and electricity usage. The economic uncertainty is the assumed discount rate used in the discounted cash flow model, and the market uncertainties are connected to the price of feedstock, electricity, utilities, and chemicals.

Each parameter was varied one at a time and the minimum selling price of dissolving pulp was calculated for each case. The results are presented in Figure 6.

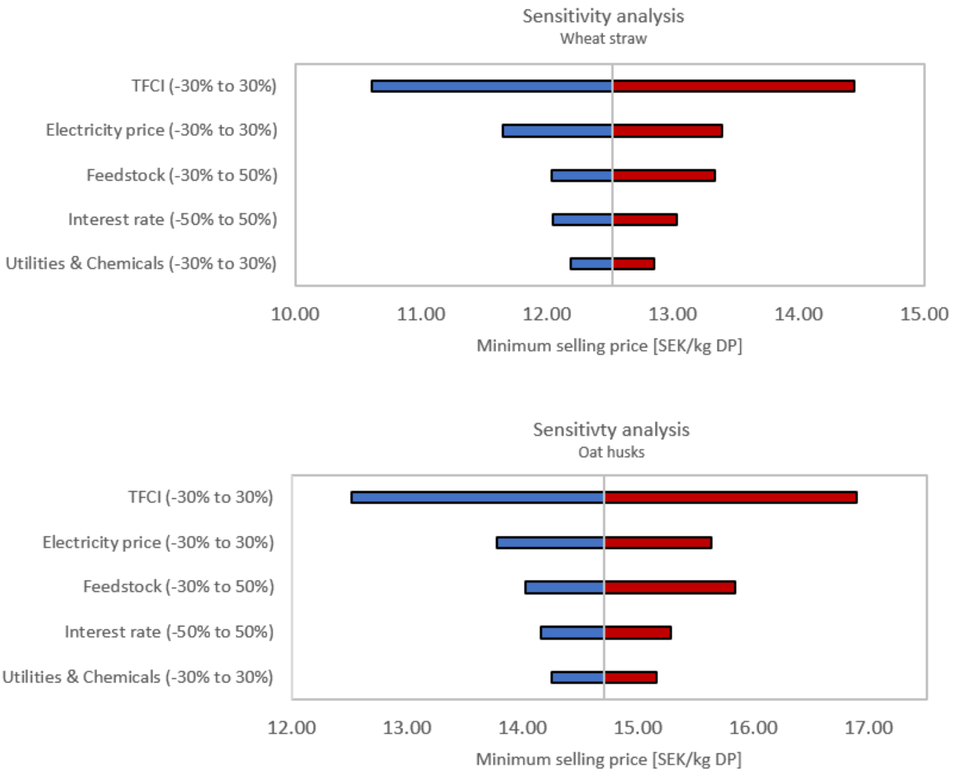

Figure 6. Tornado diagrams for single parameter sensitivity analysis of minimum selling price. Selling price of dissolving pulp indicated by industry is 10 SEK/kg DP.

The electricity price, price of utilities and chemicals as well as the TFCI was varied between -30% and 30%. Due to the uncertainty of the assumed discount rate, the discount rate was varied between -50% and 50%. The feedstock was varied between -30% and 50% due to the impact of increased interest in usage of the feedstock as well as the costs of logistics and transport, which adds 30-50% cost to the feedstock (15).

As can be seen from the sensitivity analysis, the minimum selling price for both cases show a high sensitivity to the capital investment cost. Since the simulations that was done of the two processes have a large potential of optimization, the capital investment cost could be reduced, and thus lie in the lower part of the range presented in the sensitivity analysis.

The minimum selling price for both cases show a similar, rather high, sensitivity to the change in electricity price. While both cases show a lower sensitivity to changes in utility and chemical prices. An optimization of the processes would result in a lower utility and chemical demand. This suggests that it is likely that the minimum selling price would be in the lower part of the range.

Both cases show similar sensitivity to change in interest rate and feedstock price. Since about 30-50% is added to the cost of feedstock, the price would lean toward the higher end of the range. The effect of change in interest rate does not have a large impact on the minimum selling price for any of the two cases despite the large change made to the parameter.

3.3 Environmental performance

The result from the Life Cycle Impact Assessment for the studied systems are presented in the following sections below. The results cover the base case and different sensitivity analysis studied. The sensitivity analysis studied the variation in environmental performance when using steam generated from biomass, recycling wastewater and when assigning no burden to the crop raw material. The results are reported per ton of dissolving pulp produced.

Table 5 shows that DP produced from oat husk has a higher environmental impact than that of wheat straw across all categories except in ODP where it is slightly lower.

Table 5. LCA results for oat husk and wheat straw-based pulp. The results are for the base case where the source of steam is natural gas.

Impact Category/indicator	Units	DP from wheat straw	DP from oat husk
Abiotic Depletion Potential, non- fossil resources	kg Sb eq.	0.00133	0.00153
Eutrophication Potential	kg Phosphate eq.	2.0	6.7
Photochemical Oxidant Formation Potential	kg NMVOC eq.	2.7	3.3
Total use of Renewable Primary Energy	MJ	9 800	9 550
Total use of Non-Renewable Primary Energy	MJ	31 000	30 600
Acidification Potential	Moles H+ eq.	4.15	32
Climate Change	kg CO2 eq.	1 700	1 820
Ozone Depletion Potential	kg CFC-11 eq.	1.26E-05	1.24E-05
Water Deprivation	m^3 world eq.	15.2	53

From the graph below (Figure 7) it can be observed that wheat cultivation contributes the most to the impact categories AP, EP, ODP, ADP, PERT and water deprivation, while also significantly contributing to the rest. Steam produced from natural gas dominates climate change impact while recovery boiler emissions contribute significantly to POF and AP. The production of chemicals also contributes to some of the impacts studied.

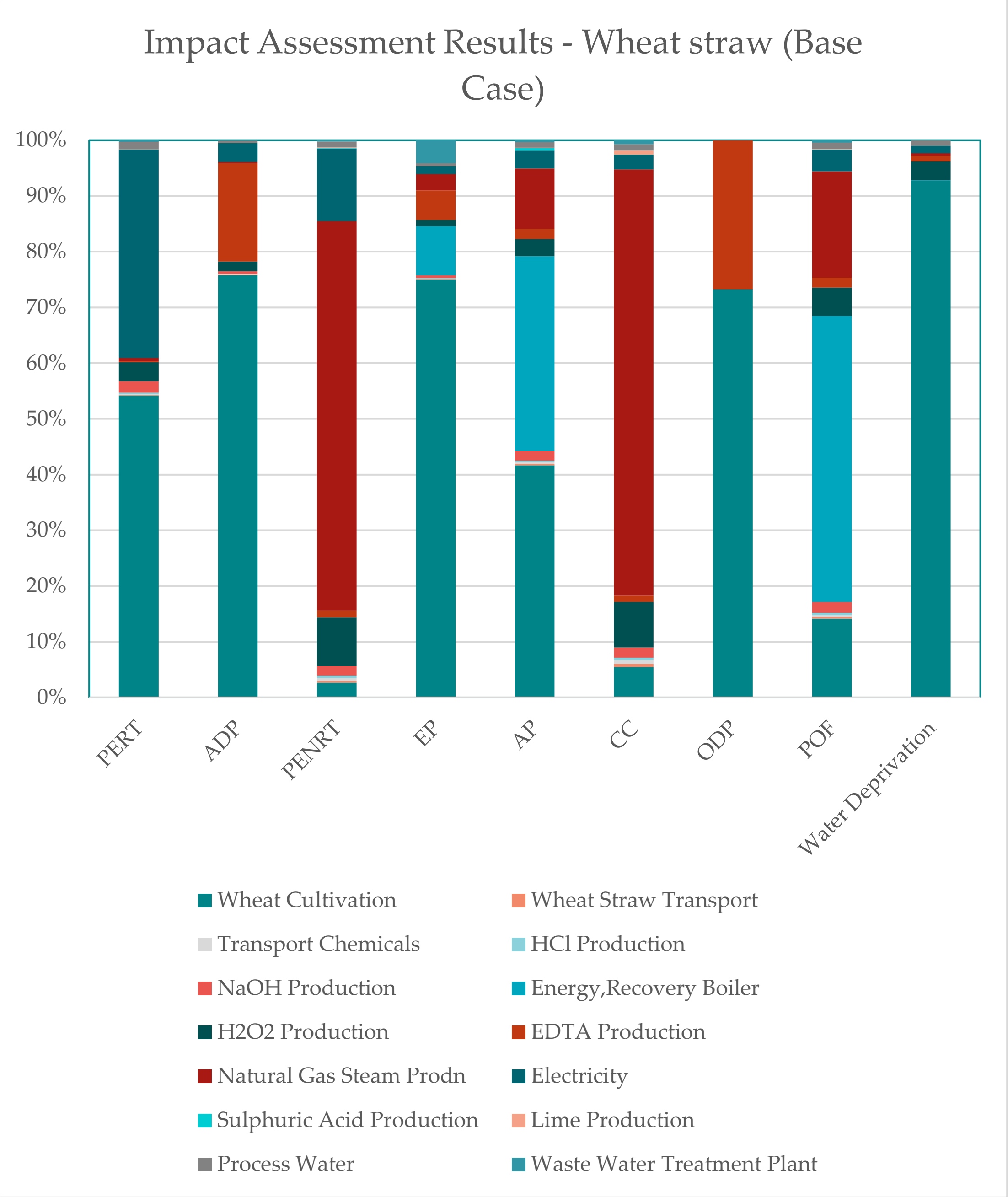

Figure 7. Contribution of activities to the different impact categories and indicators studied -wheat straw-based pulp.

The results from the impact assessment of oat husk (Figure 8) are similar to wheat straw impacts with the oat cultivation activity dominating ADP, AP, EP, ODP PERT and water deprivation, while significantly contributing to others. Emissions from the recovery boiler also have an impact, like in the wheat straw case. Steam from natural gas contributes the most to climate change impact but the production of chemicals, and cultivation of crops also contribute significantly to the climate change impact.

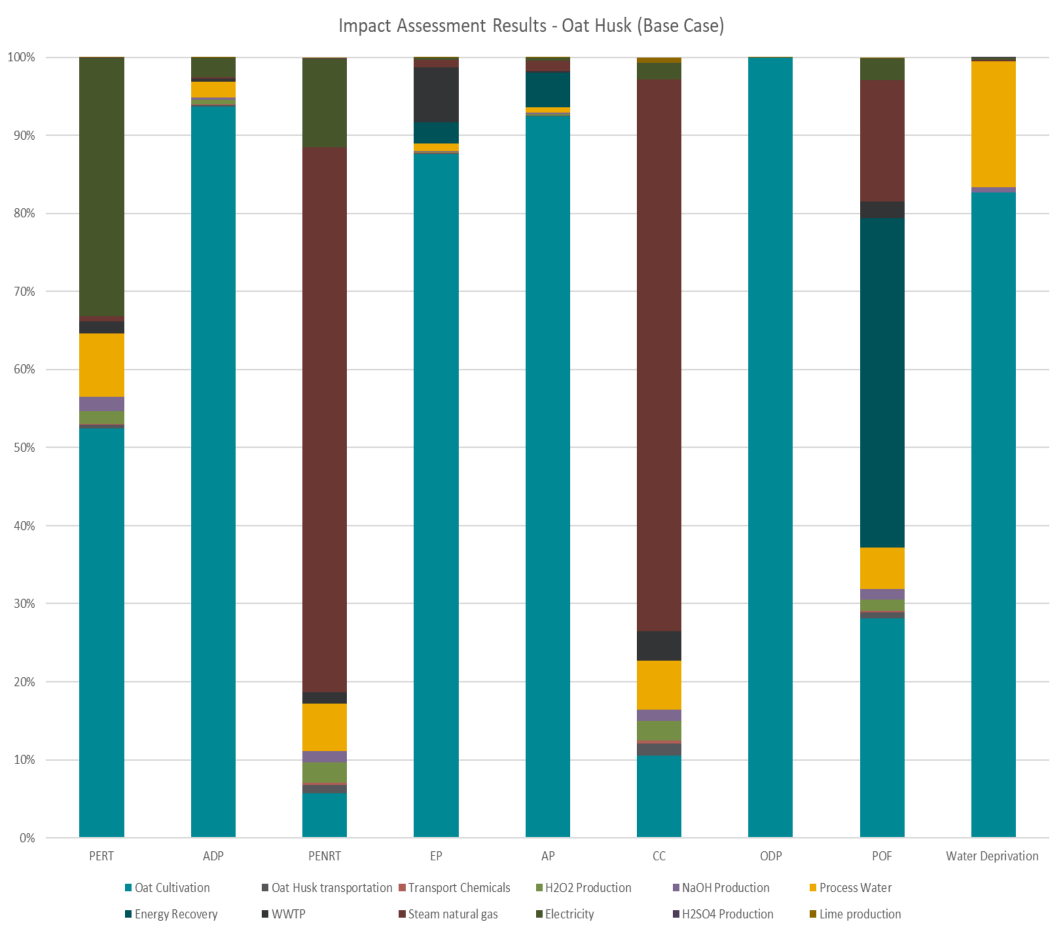

Figure 8. Contribution of activities to the different impact categories and indicators studied – oat husk-based pulp.

3.3.1.1 Climate change impact of dissolving pulp

A closer look into the climate change impact, shows that dissolving pulp from oat husk has higher impact (1820 kg CO_2 eq./ ton DP) compared to that of wheat straw (1700 kg CO_2 eq/ton DP).

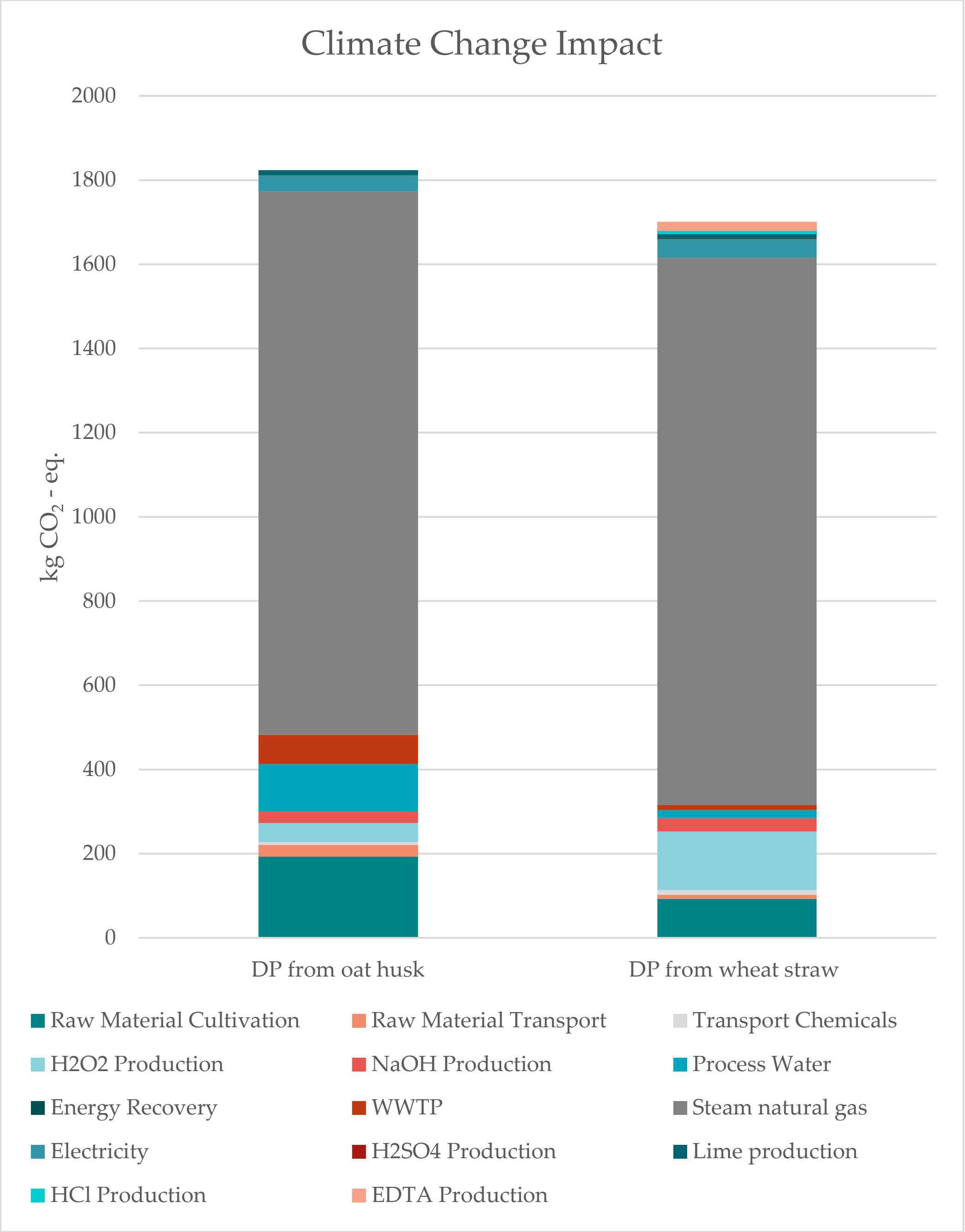

Figure 9. Comparison between oat husk and wheat straw-based pulp for Climate change impact.

3.3.2 Sensitivity analysis – steam from biomass

The result from the sensitivity analysis in changing the source of steam produced to biomass is presented in Table 6. The results show the percentage change across the indicators compared to the base case results in Table 5. It was found that the climate change impact reduces by 65% in both oat husk based and wheat straw-based pulp. It is also interesting to see that in all other impact categories/indicators the impacts increase when compared to the base case.

Table 6. LCA results for oat husk and wheat straw-based pulp showing the variation in impact categories from base case when changing the steam source to biomass.

Impact Category/indicator	% change from base case – DP from wheat straw	% change from base case – DP from oat husk
Abiotic Depletion Potential, non- fossil resources	8%	7%
Eutrophication Potential	28%	9%
Photochemical Oxidant Formation Potential	51%	39%
Total use of Renewable Primary Energy	64%	163%
Total use of Non-Renewable Primary Energy	0,5%	0
Acidification Potential	48%	6%
Climate Change	-65%	-65%
Ozone Depletion Potential	0	0
Water Deprivation	0	0

A closer look into the climate change impact of the sensitivity analysis for DP from wheat straw and oat husk can be seen in Figure 10 below. DP from wheat straw with steam from biomass has the lowest climate change impact out of the 4 cases.

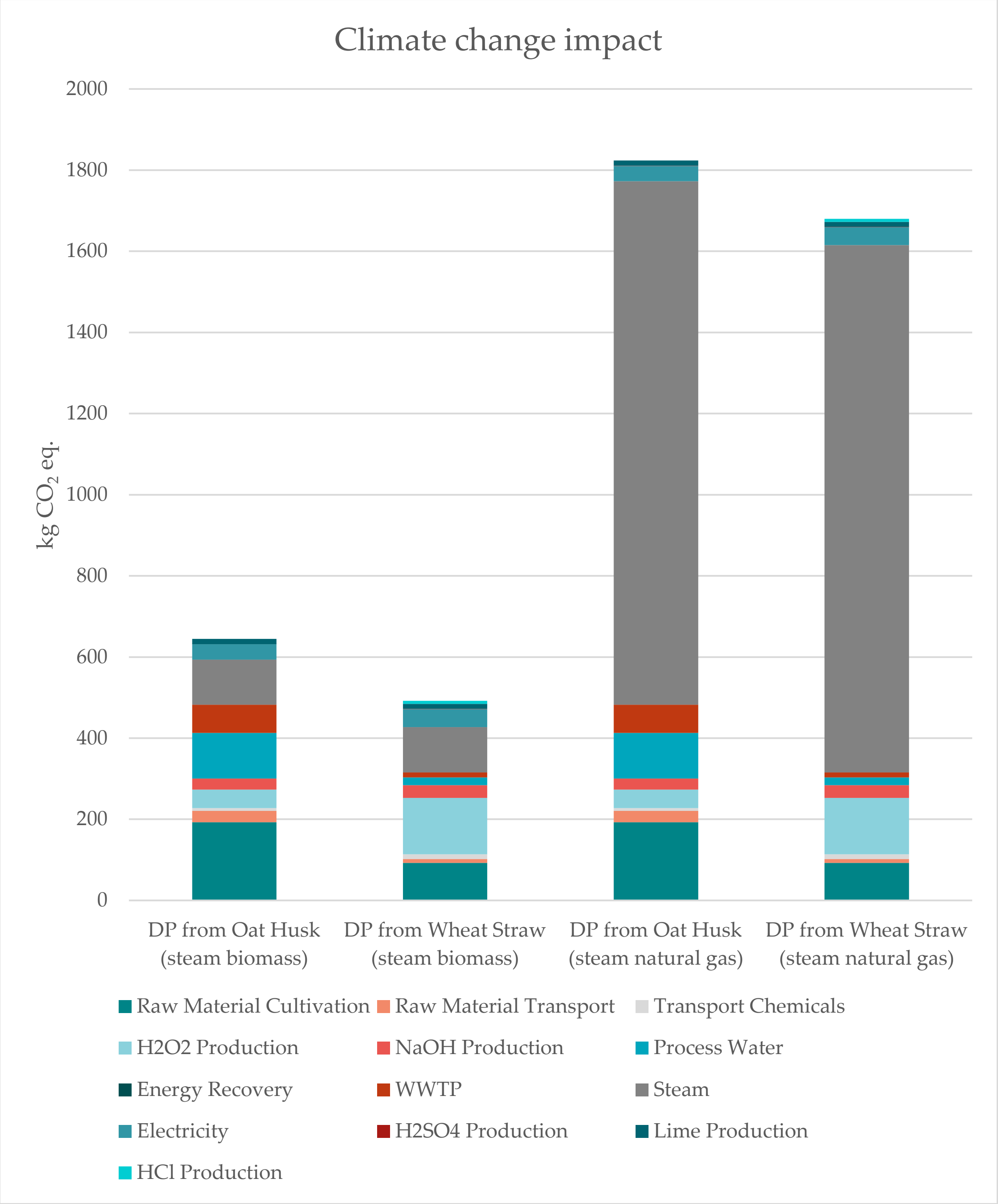

Figure 10. Comparison between oat husk and wheat straw-based pulp including sensitivity analysis for Climate change impact.

3.3.3 Sensitivity analysis – recycling of water

From literature, it was found that 60% of the water used could be recycled back to the plant (16). A sensitivity analysis was conducted to see the variation in environmental performance from the base case described.

The environmental impacts across all the categories reduces slightly (Table 7). The highest change can be observed in water deprivation, where impacts reduce by 57%. Water use for the two systems are also different. The Oat husk-based pulp uses ten times more water in its processes as compared to wheat straw-based pulp.

Table 7. LCA results for oat husk and wheat straw-based pulp showing the variation in impact categories from base case when recycling 60% of wastewater.

Impact Category	% change from base case – DP from wheat straw	% change from base case – DP from oat husk
Abiotic Depletion Potential, non- fossil resources	-0.1%	-0.74%
Eutrophication Potential	-0.2%	-0.4%
Photochemical Oxidant Formation Potential	-0.3	-3.4%
Total use of Renewable Primary Energy	-0.36	-3%
Total use of Non-Renewable Primary Energy	0	0
Acidification Potential	-0.27%	-0.3%
Climate Change	0.37%	-3%
Ozone Depletion Potential	0	0
Water Deprivation	-57%	-57%

3.3.4 Sensitivity analysis – no environmental burden allocated to the feedstock

Feedstock production has shown to contribute to a lot of the environmental impacts studied. It can be argued that since these are agricultural residues, cultivation impacts must be allocated completely to the main product and not its residues. This method of allocating environmental burden only to the main product and none to the residues is known as cut-off allocation, a common method used in LCA practice. The environmental performance of DP from wheat straw and oat husk of allocating no burden on the agricultural residues can be seen below in Table 8. There is a significant reduction across all impact categories/indicators when allocating no burden to the raw materials used.

Table 8. LCA results for oat husk and wheat straw-based pulp showing the variation in impact categories from base case when allocating no environmental burden to raw material.

Impact Category	% change from base case – DP from wheat straw	% change from base case – DP from oat husk
Abiotic Depletion Potential, non- fossil resources	-77%	-93%
Eutrophication Potential	-77%	-88%
Photochemical Oxidant Formation Potential	-15%	-27%
Total use of Renewable Primary Energy	-55%	-48%
Total use of Non-Renewable Primary Energy	-3%	0,4%
Acidification Potential	-43%	-92%
Climate Change	-7%	-12%
Ozone Depletion Potential	-73%	-100%
Water Deprivation	-98%	-83%

4 Discussion

The following section contains comments and discussion of the results of the process simulation and the techno-economic assessment as well as the life cycle impact assessment of the two cases.

4.1 Process performance

The main point to be made regarding the process performance is the simplification done during the process simulations. The oat husk process model did only include the fiber line. The chemical and utility demand of the chemical recovery cycle was approximated with the use of literature. The wheat straw process model was based on the oat husk model; however, parts of the chemical recovery cycle (the evaporators and recovery boiler) was added to this model. The caustization and calcination section of the process were simulated separately.

The wheat straw case has a higher pulping and bleaching chemical demand than the oat husk case. This is well aligned with the experimental results of Sjöstedt (3). However, the wheat straw model is more optimized than the oat husk model and it should be expected to have a better process performance than the oat husk model. This can be seen in the results of the process simulations where the process water usage of the oat husk case is almost 10 times the water demand of the wheat straw process. Further process optimization and heat integration would, most likely, result in less energy and resource intensive processes.

4.2 Economic performance

The better process performance of the wheat straw process in comparison to the oat husk process is also visible in the economic performance. Since the wheat straw process is less energy and resource intensive than the oat husk process and has a higher yield, the process it appears to be more profitable even though the price of wheat straw is higher than that of oat husk. However, it is important to keep in mind that the wheat straw process is more optimized than the oat husk process. Optimization of the processes, reducing the chemical and utility consumption, could therefore result in a more equal economic performance of the two processes.

Moreover, the two cases represent relatively small plants on an industrial scale. An increased production capacity would further decrease the production price per unit dissolving pulp due to economy of scale.

The sensitivity analysis showed that the TFCI has a large impact on the final break-even price. To reduce the relative TFCI an increased yield would be necessary. Furthermore, the cost of feedstock is one of the major operational costs and the sensitivity analysis showed that the final break-even price also was affected by the cost of feedstock. It would therefore be important to develop higher yielding chemical routes to produce dissolving pulp from wheat straw and oat husk.

Electricity, chemicals, and utility were one of the largest contributors to the cost build-up. A process optimization and further heat integration would result in a lowered cost for chemicals and utilities.

The indicated market price is 10 SEK/kg DP and by the current results both wheat straw and oat husk results in a higher total minimum selling price. However, with further optimization of the chemical routes and the processes, increased heat integration and the effect of a larger production capacity, it is possible that the minimum selling price could be decreased to below 10 SEK/kg DP and hence make the processes profitable.

4.3 Environmental Performance

It was observed that cultivation of raw material contributes significantly to the different impacts studied. Table 6 above shows that oat husk-based pulp has higher environmental impact than that of wheat straw-based pulp, especially in EP and AP. The yield for oat-based pulp is lower than that for wheat-based pulp and hence more raw material is required leading to an increase in impacts. In particular, oat cultivation activities release more nitrogen oxides and ammonia to air compared to wheat cultivation activities and hence has higher AP and EP impact. Energy recovered from recovery boiler releases sulfur dioxide and nitrogen oxides emissions to the air and hence contributes significantly to POF and AP. The use of fertilizers in cultivation could explain the high contribution towards ADP in both wheat and oat-based pulp as it uses minerals like nitrogen and potassium.

Water Deprivation potential for wheat straw-based pulp is significantly lower than that of oat husk-based pulp. This is because the process simulation data for the wheat straw-based pulp has been optimized to use less water in the overall process.

Climate Change Impact

Figure 9 from above shows that steam from natural gas is what contributes the most to the climate change impact in both cases. Along with this, cultivation and production of chemicals contribute to the climate change impact. Oat cultivation has a higher climate change impact when compared to wheat cultivation. This is possibly because of the same reason as mentioned above, lower yield. The reason for a significant impact to climate change from cultivation activities in general is due to high nitrous oxide emissions to air that occur during cultivation. Wheat straw-based pulp has higher impact to climate change from the production of hydrogen peroxide. This is due to the two-step bleaching process that is used to ensure good quality of pulp which requires more hydrogen peroxide than compared to bleaching conditions in the oat husk-based pulp.

The sensitivity analysis conducted with steam from biomass also highlight the importance of the type of steam used within the system. The processes have high energy demands and these need to be further optimized to reflect real life production, which would also affect the climate change impact studied.

4.3.1 Recycling water within the plant

The results for the sensitivity analysis show that recycling water within the plant reduces water deprivation impacts by a lot but this has only been analyzed from an environmental perspective and a techno-economic feasibility of such a provision has not been conducted. All the same it does highlight the importance of reducing water usage as much as possible within the plant and look at possible scenarios where water as a utility could be shared between different plants within the vicinity of the industry.

4.3.2 No environmental burden on agricultural residue

The sensitivity analysis conducted in allocating no burden on agricultural residue shows a significant change in environmental performance. It highlights the importance of allocation procedures for different products and how different methods can drastically affect the environmental performance of the foreground system. The datasets for cultivation are taken from generic LCA databases and assumed to be representative of oat and wheat cultivation taking place in Sweden. The environmental performance is highly sensitive to the choice of cultivation data as the results indicate, and this highlights the need for gathering specific cultivation data within Sweden so as to get comprehensive environmental performance results.

5 Conclusion

Process simulations and techno-economic and environmental impact assessment of the production of dissolving pulp (10% moisture content) from wheat straw and oat husk were performed. The key results from the study are presented below:

- The yield for the wheat straw and oat husk process was 45% and 31% respectively.
- The extra steam needed to close the energy balance, that could not be provided from heat recovery in the recovery boiler, was 7.1 and 7.0 kg/kg DP for the wheat straw and oat husk process respectively.
- The electricity demand was 2.10 and 2.25 kWh/kg DP, (94.7 GWh and 102.2 GWh), for wheat straw and oat husk.
- The largest contributor to the final price of dissolving pulp were chemicals and utility, followed by indirect costs and the cost of feedstock.
- The price for chemicals and process water was 4.00 and 4.61 SEK/kg DP for wheat straw and oat husk.
- The resulting minimum selling prices for wheat straw and oat husk were 12.5 and 14.7 SEK/kg DP (compare to 10 SEK/kg DP indicated by industry).
- Cultivation activities for feedstock (wheat straw and oat husk) have a significant impact on the environmental performance of the systems studied.
- Studying climate change impact of the production of dissolving pulp shows that oat husk-based pulp has a higher impact (1820 kg CO_2 eq./ ton DP) compared to wheat straw-based pulp (1700 kg CO_2 eq/ton DP).
- It was found that steam produced from natural gas is the highest contributor to climate change impact for both cases.
- Changing the source of steam from natural gas to biomass reduces the climate change impact by 65% for both wheat straw- and oat husk-based pulp.

Seen from a techno-economic and environmental perspective, wheat straw is showing more promising results than oat husk for the production of dissolving pulp. This is largely due to that the process of producing DP from wheat straw has a higher yield than the oat husk process. However, neither option is at the moment economically feasible.

5.1 Recommendations

The sensitivity analysis of the economic performance showed that a change in TFCI has a large impact on profitability of the processes. In order to affect the TFCI it would be important to find more optimized chemical routes to achieve higher yields. Since the cultivation of the feedstock has a significant impact on the climate impact, an increased yield would also result in a better environmental performance.

Optimization and increased heat integration would also contribute to make the process more profitable and reduce the climate impact. In addition, the effect of economy of scale would reduce the relative price of producing dissolving pulp from wheat straw and oat husk.

It is recommended to focus on finding more optimized chemical routes for the production of dissolving pulp. It is also of importance to find more optimized process and heat integration designs to make the processes less resource and energy intensive. The effect of increased production capacity on the relative price of dissolving pulp would also be of interest for further investigation.

6 Reference list

1. MEASURING FASHION 2018 Environmental Impact of the Global Apparel and Footwear Industries Study Full report and methodological considerations.

2. Preferred Fiber & Materials Market Report 2020.

3. Sjöstedt N. Isolation of cellulose fibres from agricultural waste Production of dissolving-grade pulp from oat husk and wheat straw [Internet]. Available from: www.chalmers.se

4. Ulefors A. Production of Dissolving Pulp From Oat Husks Process Design with Techno-Economic and Environmetal Assessment in a Life Cycle Perspective [Internet]. Available from: www.chalmers.se

5. Nilsson L. Soda Based Production of Dissolving Pulp from Wheat Straw Process Simulation and Techno-Economic Assessment [Internet]. Available from: www.chalmers.se

6. Mammen M. LCA of producing dissolving pulp from agricultural residue [Internet]. Available from: www.chalmers.se

7. Skotte E, Åkesson E. Organosolv using Wheat Straw Dissolving Pulp Production and Process Simulation [Internet]. Available from: www.chalmers.se

8. Das PK, Das BP, Dash P. Potentials of postharvest rice crop residues as a source of biofuel. In: Refining Biomass Residues for Sustainable Energy and Bioproducts: Technology, Advances, Life Cycle Assessment, and Economics. Elsevier; 2019. p. 275–301.

9. Kapoor M, Panwar D, Kaira GS. Bioprocesses for Enzyme Production Using Agro-Industrial Wastes: Technical Challenges and Commercialization Potential. In: Agro-Industrial Wastes as Feedstock for Enzyme Production: Apply and Exploit the Emerging and Valuable Use Options of Waste Biomass. Elsevier Inc.; 2016. p. 61–93.

10. Schmitz E, Nordberg Karlsson E, Adlercreutz P. Warming weather changes the chemical composition of oat hulls. Plant Biol. 2020 Nov 1;22(6):1086–91.

11. Piccinno F, Hischier R, Seeger S, Som C. From laboratory to industrial scale: a scale-up framework for chemical processes in life cycle assessment studies. J Clean Prod. 2016 Nov 1;135:1085–97.

12. Towler GP, Sinnott RK. Chemical engineering design : principles, practice, and economics of plant and process design. Butterworth-Heinemann; 2013. 1303 p.

13. Mesfun S, Matsakas L, Rova U, Christakopoulos P. Technoeconomic assessment of hybrid organosolv-steam explosion pretreatment of woody biomass. Energies (Basel). 2019;12(21).

14. Seider W. D. Lewin D. R. Seader J. D. Widagdo S. Gani R. & Ng K. M. Product and process design principles: synthesis analysis and evaluation (Fourth). John Wiley & Sons; 2017.

15. Searcy E, Flynn P, Ghafoori E, Kumar A. The Relative Cost of Biomass Energy Transport. 2007.

16. Alexandersson T. Water Reuse in Paper Mills: Measurements and Control Problems in Biological Treatment. 2003;

17. Ek Monica, Gellerstedt G, Henriksson Gunnar. Pulp and paper chemistry and technology. Volume 2, Pulping chemistry and technology. Walter de Gruyter; 2009. 471 p.

18. Sanchez DR. RECAUSTICIZING-PRINCIPLES AND PRACTICE.

19. Förstudie: Eldriven kalcinering.

20. Kok JS, Ng S, Martinez E. Design, Integration and Sustainability Analysis Biorefineries and Chemical Processes.

21. Sandin G, Zetterberg TS, Rydberg T. Tillgång på skogsråvara-sammanfattning och scenarier en förstudie [Internet]. 2019. Available from: www.ivl.se

Appendix A. Lime-cycle calculations

In the following appendix the simulation and techno-economic assessment of the lime-cycle for the wheat straw case is presented. The costs of are thereafter scaled to obtain the costs for the oat husk case by using the wheat straw case as reference.

Process simulations

In the simulation the electrolyte NRTL method was used. The flowchart of the process is presented in Figure A1.

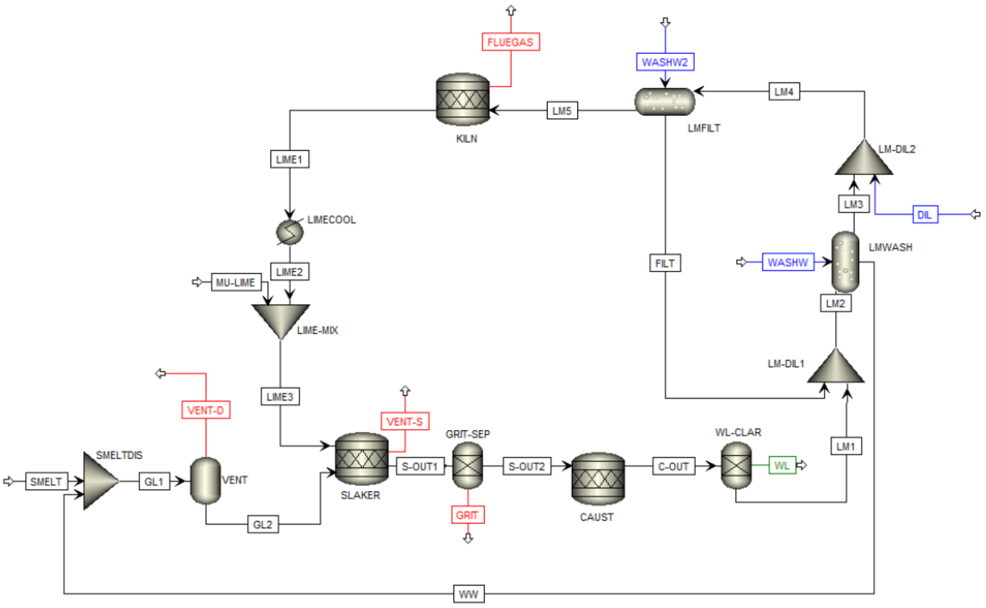

Figure A1. Flowchart of the lime-cycle simulated in Aspen PLUS.

Smelt Dissolver

The smelt dissolver was simulated as a mixer and a flash. In the mixer, weak white liquor from the lime mud washer was combined with an input stream of salts. The flash was setup with zero pressure change and zero duty so that vapor produced in the mixing would be separated. The input stream of salts was set based on the amount of sodium hydroxide entering the recovery boiler in a previously performed simulation done by Nilsson (5). Only NaOH and Na_2CO_3 was assumed to be present in the salt stream. The amount of weak wash was adjusted by setting the amount of wash water in the lime wash with a design specification so that the concentration of the salts in the green liquor would be in the range for a typical kraft mill, see Table A1.

Table A1. Approximate concentrations of salts in green liquor (17)

Salt/ion	Na	K	Na_2CO_3	Na_2S	NaOH	Na_2SO_4	$Na_2S_2O_3$	NaCl
Conc. [g/kg]	70-95	5-15	100-140	30-60	2-25	1-15	1-10	1-10

Slaking and Causticizing

In the slaker and causticizers the following reactions take place,

$$CaO(s) + H_2O \rightarrow Ca(OH)_2(s) \tag{I}$$

$$Ca(OH)_2(s) \leftrightarrow CaCO_3(s) + 2OH^- \tag{II}$$

The slaker was modelled as a stoichiometric reactor were the conversion of Reaction I was 99% and the conversion of Reaction II was 75%. The duty of the reactor was set to 0. There were 2 exit streams from the reactor, one for vapor and one for liquid and solids. The amount of lime entering the slaker was set with a design specification which varied the make-up lime so that, on a molar basis, there would be 1.1 times the amount of Na_2CO_3 of CaO entering the slaker.

To simulate the removal of grits formed in the slaking process a separator was used. It was assumed that 90% of the unreacted CaO, 1% of the formed $Ca(OH)_2$ and 1% of the formed $CaCO_3$ would be removed from the process in the form of grits. The amount of liquor removed in the separation of grits was set by a calculator so that the grits would consist of 75 wt-% solids (18).

Reaction II is an equilibrium reaction that can be described by

$$K = \frac{[OH^-]^2}{[CO_3^{2-}]}(s) \tag{A1}$$

The equilibrium ratio is dependent on the ion strength in the liquor as can be seen in Figure A2. In a typical kraft mill the ion strength is around 4 mole/kg (17).

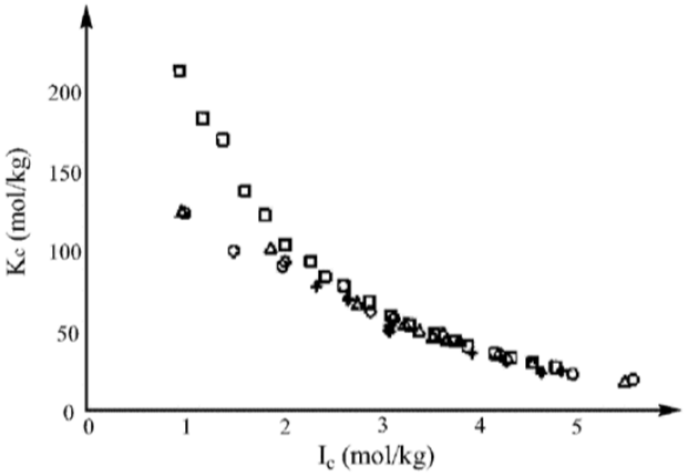

Figure A2. The equilibrium of reaction II against ion strength (17).

The equilibrium can also be described as

$$\ln K_C = \left[A_C + \frac{B_C}{T}\right] + \left[C_C + \frac{D_C}{T}\right] \times I_C^{n_C} \qquad (A2)$$

where K_C is equilibrium ratio in mole/kg, *A*-*D* are empirical constants, *n* is an empirical constant, *T* is the temperature in K and *I* is the ion strength. The numerical values of the empirical constants can be seen in Table A2

Table A2. Numerical values of the constants in equation A2 (17).

Parameters	Value
n_C	1.15
A_C	2.67
B_C	915
C_C	-0.074
D_C	-82.4

The causticizing vessels were modelled as a stoichiometric reactor. The conversion of Reaction II was set by using a calculator and a design specification. In the calculator the equilibrium ratio, *K*, was calculated based on the ionic strength according to Equation A2. The design specification varied the fractional conversion in the reactor so that the conditions of Equation A1 was met.

White Liquor Clarification

The white liquor clarification was simulated as a separator, all solid components went to the lime mud stream and with a design spec. the fraction of liquor entering the lime mud stream was set so that the wt-% of solids in the lime mud would be 40% (18).

Before the lime mud wash, the lime mud stream was diluted with the filtrate from the lime mud filter using a mixer. The washer was simulated as a washer were the L:S ratio was set to 1.22 so that the wt-% of solids exiting the washer would be 45%. The amount of wash water was set with a design specification so that the concentration of the salts in the green liquor would be in the range for a typical kraft mill, see Table A1.

Between the washer and the filter, the lime mud was diluted to 25 wt-% solids with water using a mixer. The filter was simulated as a washer with a L:S ratio of 0.333 so that the solids in the discharge would be 75 wt-%. The amount of wash water was 1.5 the liquor in the discharge which was specified with a calculator. In both washers the mixing efficiency was assumed to be 1.

The L:S ratios and inlet temperatures in the different stages of the lime mud washing is based on typical values for recausticizing plants as presented by Sanchez (18).

Lime Kiln

The lime kiln was simulated as a stoichiometric reactor. In the kiln the method was changed to the NRTL method. The reactions in the kiln were,

$$Ca(OH)_2(s) \rightarrow CaO(s) + H_2O \qquad (III)$$

$$CaCO_3(s) \rightarrow CaO(s) + CO_2 \qquad (IV)$$

The exit temperature for the reactor was set to 1000°C. In the reactor it was specified that all vapors would enter the flue gas stream and all liquids and solids would enter the lime stream. The conversion of Reaction III was assumed to be 99% and the conversion of Reaction IV was assumed to be 90%.

The reburned lime was cooled to 50°C before being combined with a make-up lime stream in a mixer. The amount of make-up lime needed was specified with a design specification as described earlier.

Economic evaluation

The sizing of most of the process units was based on the flow rates and equipment loading rates found in Table A3

Table A3. Equipment loading rates (18)

Equipment	Unit	Value
Raw Green Liquor Stabilization	H	2-4
Green Liquor Clarifier	m/h	0.4-0.55
Slaker (clarifiers)	min	10-15
Causticizers (clarifiers)	min	90
White Liquor Clarifier (Unit type)	m^2/ton/day	0.92-1
Lime Mud Washer (Unit type)	m^2/ton/day	0.72-0.82
Lime Mud Filter	ton/day/m^2	5.9-7.3

The cost of the different process units was estimated by the same method used in Section 2.2. The cost of the smelt dissolver, green liquor stabilizer, green liquor clarifier, white liquor clarifier, lime mud washer, lime mud storage and lime mud filter were calculated as cone roof tanks. The slaker and causticizers were costed as jacketed and agitated reactors. It was assumed that 4 caustizing vessels were needed.

Table A4. Costing parameters used for economic evaluation of the lime-cycle equipment. Parameters refer to parameters used in Equation 1.

Equipment	Unit for size, S	a	b	c
Single Stage Centrifugal Pump	Flow, l/s	8000	240	0.9
Jacketed, Agitated Reactor	Volume, m^3	61 500	32 500	0.8
Cone Roof Tank	Capacity, m^3	5800	1600	0.7

The cost of the plasma generator used for burning the lime was estimated by using the work of Bjotveit et al. (19) as reference and scale it, using Equation 3. The reference data for the costing calculation was a plasma generator with 3 MW capacity with the price of 9 MSEK.

Economic evaluation

The total fixed capital cost of the lime-cycle as well as the fixed operational costs were estimated by the same method that was described in Section 2.2. The variable operating costs were calculated by using the prices presented in Table A5 and the data from the simulation.

Table A5. Prices used to calculate operating costs for the lime-cycle.

Input	Cost	Unit	Source
Process water	0.01	SEK/kg	Estimated from (12)
CaO	1.38	SEK/kg	(16)
Electricity	1378	SEK/MWh	Cost 2022 in area SE3. (17)

The capital and operating costs for the white liquor preparation plant for the wheat straw and oat husk cases can be seen in Table A6. The plant produces 3.71 t NaOH/h with a concentration of 9.4 wt-%.

Table A6. Capital and operational costs for the lime-cycle for the wheat straw and oat husk case.

Cost	Wheat straw	Oat husk
Capital cost		
Cost of major equipment [MSEK]	109.9	126.4
TFCI [MSEK]	474.6	546.2
Variable operating costs		
Process water [MSEK/year]	3.18	4.02
CaO [MSEK/year]	0.66	0.83
Electricity [MSEK/year]	69.03	87.25
Total [MSEK/year]	72.87	92.1

The variable operating costs were scaled from the wheat straw case to the oat husk case by assuming that the same amount of electricity, CaO and process water per kg dry solids were required in both cases. The amount of dry solids entering the recovery boiler was 2.49 kg DS/s and 3.03 kg DS/s for the wheat straw and oat husk case respectively.

The cost of major equipment for the oat husk case was estimated using Equation 3 where *Capacity 1* and *Capacity 2* were set to the amount of dry solids entering the recovery boiler in the wheat straw and oat husk case respectively and *Cost 1* was the major equipment cost for the lime-cycle of the wheat straw case.

Appendix B. Economic parameters

Parameters	Value	Unit	Remark	References
Variable operating costs				
Feedstock				
Wheat straw	0.73	SEK/kg	2022	(5)
Oat husk[1]	0.71	SEK/kg	2022	(10)
Utilities & chemicals				
Process water	0.01	SEK/kg		(5)
Hydrochloric acid (HCL)	1.53	SEK/kg		(5)
Sulfuric acid (H_2SO_4)	5.99	SEK/kg		(5)
Sodium hydroxide (NaOH)	6.13	SEK/kg		(5)
Calcium oxide (CaO)	1.38	SEK/kg		
EDTA	39.2	SEK/kg		(5)
Hydrogen peroxide (H_2O_2)	4.57	SEK/kg		(5)
Electricity	1378	SEK/MWh		(5)
Steam	0.01	SEK/kWh		(5)
Fixed operating costs				
Labor costs				
Number of staff	20			(20)
Wages per employee	35 000	SEK/month		(20)
Factor for allowance/overhead	1.45			(20)
Labor cost	12 180 000	SEK/year		(20)
Supervision	20	%	% Total labor costs	(20)
Total labor cost	-	SEK/year	Labor cost + Supervision	(20)
Operation and maintenance (O&M)	5	%	% of TFCI	(20)
Indirect costs				
Laboratory cost	20	%	% of Total labor costs	(20)
Plant overheads	20	%	% of Total labor costs	(20)
Capital charges	10	%	% of TFCI	(20)
Insurance	1	%	% of TFCI	(20)
Taxes	2	%	% of TFCI	(20)
Royalties	1	%	% of TFCI	(20)
Others	20	%	% of total labor cost + indirect cost	(20)
Other parameters				
Discount rate	10	%		
Plant life time	10	Years		
Market price of dissolving pulp (DP)[2]	10 000	SEK/Adt		(4)

1. The cost of oat husks is estimated based on the cost of forest residues for fuel production presented the work of Sandin, Zetterberg, and Rydberg (21).
2. From discussion with industry, a market price of around 10 000 SEK per ton of dry weight pulp was indicated (4).

Appendix C. Economic evaluation

Tabel A1. Economic evaluation of oat husk for production of dissolving pulp.

	Year	**2023**	**2024**	**2025**	**2026**	**2027**
	Production [kg]	13 632 900	31 810 100	45 443 000	45 443 000	45 443 000
Investment	Capital investment [SEK]	347 197 967	433 997 459	86 799 492		
	Discounted capital investment [SEK]	347 197 967	394 543 144	71 735 117		
	Interest on capital [SEK]	34 719 797	72 300 522	74 937 509	69 419 070	63 348 788
	Working capital [SEK]			43 399 746		
Production cost	Feedstock [SEK]	31 027 200	72 396 800	103 424 000	103 424 000	103 424 000
	Utilities and chemicals [SEK]	62 816 554	146 571 959	209 388 513	209 388 513	209 388 513
	Labor cost [SEK]	4 384 800	10 231 200	14 616 000	14 616 000	14 616 000
	O&M [SEK]	13 019 924	30 379 822	43 399 746	43 399 746	43 399 746
	Other [SEK]	11 064 422	25 816 985	36 881 407	36 881 407	36 881 407
	Indirect costs [SEK]	37 917 387	88 473 902	126 391 288	126 391 288	126 391 288
	Minimum selling price [SEK]					
Evaluation	Sales [SEK]	200 701 750	468 304 083	669 005 833	669 005 833	669 005 833
	Net Earnings [SEK]	40 471 464	94 433 415	134 904 879	134 904 879	134 904 879
	Cash flow (PV) [SEK]	-306 726 503	-339 564 043	4 705 641	134 904 879	134 904 879
	Discounted Cash Flow [SEK]	-306 726 503	-308 694 585	3 888 960	101 356 032	92 141 848
	Cumulative DCF [SEK]	-306 726 503	-615 421 088	-611 532 128	-510 176 096	-418 034 248

	Year	**2028**	**2029**	**2030**	**2031**	**2032**	**2033**		Per kg DP
	Production [kg]	45 443 000	45 443 000	45 443 000	45 443 000	45 443 000	45 443 000		
Investment	Capital investment [SEK]								
	Discounted capital investment [SEK]								1.79
	Interest on capital [SEK]	56 671 477	49 326 435	41 246 890	32 359 389	22 583 139	11 829 263		1.16
	Working capital [SEK]						-43 399 746		0
Production cost	Feedstock [SEK]	103 424 000	103 424 000	103 424 000	103 424 000	103 424 000	103 424 000		2.28
	Utilities and chemicals [SEK]	209 388 513	209 388 513	209 388 513	209 388 513	209 388 513	209 388 513		4.61
	Labor cost [SEK]	14 616 000	14 616 000	14 616 000	14 616 000	14 616 000	14 616 000		0.32
	O&M [SEK]	43 399 746	43 399 746	43 399 746	43 399 746	43 399 746	43 399 746		0.96
	Other [SEK]	36 881 407	36 881 407	36 881 407	36 881 407	36 881 407	36 881 407		0.81
	Indirect costs [SEK]	126 391 288	126 391 288	126 391 288	126 391 288	126 391 288	126 391 288		2.78
	Minimum selling price [SEK]								**14.71**
Evaluation	Sales [SEK]	669 005 833	669 005 833	669 005 833	669 005 833	669 005 833	669 005 833		
	Net Earnings [SEK]	134 904 879	134 904 879	134 904 879	134 904 879	134 904 879	134 904 879		
	Cash flow (PV) [SEK]	134 904 879	134 904 879	134 904 879	134 904 879	134 904 879	178 304 625		
	Discounted Cash Flow [SEK]	83 765 316	76 150 287	69 227 534	62 934 122	57 212 838	68 744 152		
	Cumulative DCF [SEK]	-334 268 932	-258 118 645	-188 891 111	-125 956 989	-68 744 152	**0**		**NPV = 0**

Tabel A2. Economic evaluation of wheat straw for production of dissolving pulp.

	Year	**2023**	**2024**	**2025**	**2026**	**2027**
	Production [kg]	13 542 198	31 598 461	45 140 658	45 140 658	45 140 658
Investment	Capital investment [SEK]	301 524 045	376 905 056	75 381 011		
	Discounted capital investment [SEK]	301 524 045	342 640 960	62 298 356		
	Interest on capital [SEK]	30 152 405	62 789 382	65 079 473	60 286 986	55 015 249
	Working capital [SEK]			37 690 506		
Production cost	Feedstock [SEK]	21 934 358	51 180 169	73 114 528	73 114 528	73 114 528
	Utilities and chemicals [SEK]	54 102 868	126 240 025	180 342 893	180 342 893	180 342 893
	Labor cost [SEK]	4 384 800	10 231 200	14 616 000	14 616 000	14 616 000
	O&M [SEK]	11 307 152	26 383 354	37 690 506	37 690 506	37 690 506
	Other [SEK]	9 762 715	22 779 669	32 542 384	32 542 384	32 542 384
	Indirect costs [SEK]	33 121 625	77 283 791	110 405 416	110 405 416	110 405 416
	Minimum selling price [SEK]					
Evaluation	Sales [SEK]	169 760 957	396 108 900	565 869 857	565 869 857	565 869 857
	Net Earnings [SEK]	35 147 439	82 010 692	117 158 131	117 158 131	117 158 131
	Cash flow (PV) [SEK]	-266 376 606	-294 894 365	4 086 614	117 158 131	117 158 131
	Discounted Cash Flow [SEK]	-266 376 606	-268 085 786	3 377 367	88 022 638	80 020 580
	Cumulative DCF [SEK]	-266 376 606	-534 462 392	-531 085 025	-443 062 387	-363 041 808

	Year	**2028**	**2029**	**2030**	**2031**	**2032**	**2033**		Per kg DS
	Production [kg]	45 140 658	45 140 658	45 140 658	45 140 658	45 140 658	45 140 658		
Investment	Capital investment [SEK]								
	Discounted capital investment [SEK]								1.57
	Interest on capital [SEK]	49 216 340	42 837 539	35 820 858	28 102 509	19 612 325	10 273 123		1.02
	Working capital [SEK]						-37 690 506		0
Production cost	Feedstock [SEK]	73 114 528	73 114 528	73 114 528	73 114 528	73 114 528	73 114 528		1.62
	Utilities and chemicals [SEK]	180 342 893	180 342 893	180 342 893	180 342 893	180 342 893	180 342 893		4.00
	Labor cost [SEK]	14 616 000	14 616 000	14 616 000	14 616 000	14 616 000	14 616 000		0.32
	O&M [SEK]	37 690 506	37 690 506	37 690 506	37 690 506	37 690 506	37 690 506		0.84
	Other [SEK]	32 542 384	32 542 384	32 542 384	32 542 384	32 542 384	32 542 384		0.72
	Indirect costs [SEK]	110 405 416	110 405 416	110 405 416	110 405 416	110 405 416	110 405 416		2.45
	Minimum selling price [SEK]								**12.54**
Evaluation	Sales [SEK]	565 869 857	565 869 857	565 869 857	565 869 857	565 869 857	565 869 857		
	Net Earnings [SEK]	117 158 131	117 158 131	117 158 131	117 158 131	117 158 131	117 158 131		
	Cash flow (PV) [SEK]	117 158 131	117 158 131	117 158 131	117 158 131	117 158 131	154 848 636		
	Discounted Cash Flow [SEK]	72 745 982	66 132 711	60 120 646	54 655 133	49 686 484	59 700 853		
	Cumumalitve DCF [SEK]	-290 295 826	-224 163 115	-164 042 470	-109 387 337	-59 700 853	**0**		**NPV = 0**

Appendix D. Estimation of equipment costs

The simulations of the wheat straw case included the chemical and energy recovery cycle. This section was not included in the oat husk case. Therefore, it was necessary to estimate the size and cost of the equipment of the recovery cycle, as well as the pulp drying section, for the oat husk case. The two cases have the same process layout. The results from the equipment sizing and cost calculations could therefore be used to estimate the cost of the same equipment and utility usage for the oat husk case. Table D1 shows the capacities and the corresponding values used for the estimation as well the resulting costs and energy demands.

Table D1. Result from the equipment sizing and cost calculations for the oat husk case, estimated from the wheat straw case.

	Boiler	**Evaporators (5 effects)**	**Dryer**	**Dryer: Electricity**	**Dryer: Steam**
Base for estimation	Amount of steam produced (kg/s)	Amount of water evaporated (kg/s)	Amount dry product (ADt/yr)	Demand of electricity for evaporation (1050 kWh/ton)	Demand of electricity for evaporation (1056 kWh/ton)
Size: Wheat straw[a]	6.04 kg/s	25.98 kg/s	45141 ADt/yr	5229 kW	5259 kW
Size: Oat husk[a]	7.00 kg/s	35.20 kg/s	45443 ADt/yr	4544 kW	4570 kW
Cost: Wheat straw[b]	9.35 MSEK	13.81 MSEK	3.56 MSEK	-	-
Estimated cost: Oat husk	10.22 MSEK	16.30 MSEK	4.20 MSEK	-	-

a. Used as *capacity* in Equation 3

b. Used as *cost* in Equation 3

Appendix E. LCA methodology and assumptions

This section outlines the important methodologies and assumptions made in the LCA study. More information on these assumptions can be found in (5,6). A few changes have been made to the DP from oat husk LCA in order to harmonize the method with the method used in the LCA of the DP from wheat straw.

Goal and Scope

The goal of this LCA was to investigate the environmental impacts of producing dissolving pulp from oat husk and wheat straw as raw material via the soda cooking process. The scope of the study is a cradle to gate prospective attributional LCA in which the processing of all chemicals required, raw materials along with their transport up to the point where dissolving pulp leaves the gate of the industry is considered.

Functional Unit

The functional unit of this LCA is 1 ton of dissolving pulp produced. This was assumed to be appropriate as the function of the system studied is to produce dissolving pulp and quantifying impacts. The functional unit does not account for the difference in quality of pulp produced from the different raw materials.

System boundaries

The system boundary along with activities included and excluded can be seen in Fig 2 in chapter 2.

Geographical Boundaries

The plants are assumed to be set up in Nymölla, Skåne county, Sweden as TTT has an existing pilot plant present. Raw materials are assumed to be sourced from within the county and chemicals required are assumed to be supplied from Europe.

Time Horizon

The production of the plant is assumed to begin 5 years from now with an operational life of 10-12 years. Aspects related to how chemicals, energy and raw materials are produced 5 years from now are not captured. The processes in place today are assumed to be in place 5 years into the future.

Other Boundaries

Capital goods and personnel are not included in this study. Construction impacts are not included in this study as well as including them will have no difference in impact to the product under study.

Life Cycle Inventory Analysis

Data required for the LCA were mainly supplemented with data from the process modelling and simulation of the processes. Table E.1 below shows the inventory data for the entire process modelled in the software LCA for experts (formerly GaBi). More information datasets can be found in the work done by Parayil (6).

Table E1. Lifecycle inventory analysis for both wheat straw and oat husk based dissolving pulp.

Materials	Units	Wheat straw based pulp	Oat husk based pulp
Inputs			
Raw Material	kg/ton DP	2215.33	3200
Sulphuric Acid	kg/ton DP	2.91	2.47
Sodium Hydroxide	kg/ton DP	36.47	214.23
Hydrogen Peroxide	kg/ton DP	84.94	39.74
EDTA	kg/ton DP	4.85	-
Hydrochloric Acid	kg/ton DP	32.56	-
Lime	kg/ton DP	10.53	10.53
Process Water	kg/ton DP	17989.77	104017
Steam	MJ/ton DP	18489.7	18299.8
Electricity	MJ/ton DP	3550.55	3061.06
Outputs			
Dissolving Pulp	ton	1	1
Emissions			
Sulphur di oxide	kg/ton DP	0.362	0.362
Total Reduced Sulphur	kg/ton DP	0.2	0.2
Nitrogen oxides	kg/ton DP	1.365	1.365
Particulates	kg/ton DP	0.81	0.81

Table E2. List of Datasets used for the different activities in LCA modelling.

Material	Dataset
Wheat Straw	Wheat production in Switzerland CH: Wheat production, Swiss integrated production, extensive
Oat Husk	Oat Production in Finland
EDTA	EDTA production in Europe
Hydrochloric Acid	HCl production (100%) in Germany
Hydrogen Peroxide	Hydrogen peroxide (100%), steam cracking production in Germany
Sodium Hydroxide	Sodium hydroxide (caustic soda) mix (100%) in EU
Sulphuric Acid	Sulphuric acid (96%) production in EU
Lime	Lime production in Germany
Electricity	Electricity grid mix 1kV-60kV Sweden
Process Water	Process water from surface water within EU
Steam	Process steam from natural gas 90% within Sweden
Steam (sensitivity analysis)	Process steam from biomass (solid) 90% within Sweden

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