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Sustainable production of Cellulose-based products and additives to be used in SMEs and rural areas

Deliverable D2.2. Mathematical tools in small biorefineries: artificial neural network models, simulation and optimization and LCA

CELISE: Sustainable production of Cellulose-based products and additives to be used in SMEs and rural areas

Deliverable D2.2. Mathematical tools in small biorefineries: artificial neural network models, simulation and optimization and LCA

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LIST OF ABBREVIATIONS

TEA: Techno-economic analysis

LCA: Life cycle assessment

HVACs: High value-added chemicals

CAPEX: Capital expenditures

OPEX: Operational expenditures

1. SUMMARY

This report presents the results of various studies performed for the three tasks (Tasks 2.2, 2.3, 2.4) under WP2 of CELISE project in the areas of Artificial neural network models, simulation and optimisation and LCA. The studies were performed during the various secondments under CELISE and/or from internal work of the partners. In brief, 2 studies were presented in Artificial Neural Networks (ANNs), 6 studies on Simulation and optimisation (including techno-economic analyses and feasibility studies) and 5 studies on LCA (including feasibility studies containing environmental data) including a methodology of transfering LCA knowledge to rural areas. The titles of the studies presented are listed below

1. **Artificial Neural Networks**

    a) Artificial Neural Networks Modelling in steam explosion pre-treatment.
    b) Artificial Neural Networks Modelling in hydrothermal pre-treatment.

2. **Simulation and optimisation**

    a) Case 1: Process modelling of barley's spent grain to bioethanol.
    b) Case 2: Process modelling of Algae (Ulva rigida) to different valorisation options.
    c) Case 3: Feasibility study of lignocellulosic loose-fill thermal insulation material using steam explosion technology.
    d) Case 4: Techno-economic analysis of the production of phenolic and furanic fractions/compounds from biomass.
    e) Case 5: Techno-economic analysis of Kraft lignin fast (catalytic) pyrolysis for the production of high value-added chemicals (HVACs).
    f) Case 6: Process modelling of chitosan production from dead bees.

3. **Life cycle assessment**

    a) Case 1: LCA of bioethanol production from brewer's spent grain.
    b) Case 2: Feasibility study (with environmental data) for egg packaging from ecological and biodegradable materials from natural fibres with functional biopolymer additives.
    c) Case 3: LCA of HVACs production from lignin pyrolysis.
    d) Case 4: LCA of chitosan production from dead bees (bases on initial results).
    e) Case 5: Methodology for transferring knowledge regarding LCA to non-developed rural areas (La Guajira).

A concise description of the procedures, analysis and outcomes is described in the next chapters.

2. INTRODUCTION

2.1. General purpose of the document

This document consists of 3 parts presenting the results of artificial neural network modelling, process simulation and techno-economic analyses and life cycle assesments, performed under the project CELISE

2.2. Role and contribution from partners

The D2.2 is part of WP2 activities and UCC leads it. In this case, AUTH has been the main responsible of this deliverable; however, the deliverable joins all of the activities related to the neural network modelling, process simulation and techno-economic analyses and life cycle assesments, pyrolysis, and the following partners are involved in these activities: UC (Universidad de Cantabria), UPM (Universidad Politécnica de Madrid), LSIWC (Latvian State Institute of Wood Chemistry), AUTH (Aristotle University of Thessaloniki), UTB (Univerzita Tomase Bati ve Zline), CVUT (Ceske Vysoke Uceni Technicke v Praze), UNACH (Universidad Nacional de Chimborazo), UNL-FICH (Universidad Nacional del Litoral) and Latitud (Latitud-Fundación Laboratorio Tecnológico del Uruguay).

3. PART A – ARTIFICIAL NEURAL NETWORK MODELLING (TASK 2.3)

3.1. Introduction to Artificial Neural Networks (ANNs)

Artificial Neural Networks (ANNs) are a powerful modeling tool that has seen significant development in recent years, mainly due to the increased computational capacity of modern computers. ANNs have been applied across a wide range of fields, from medicine to finance. Based on the developed neural network, the relationships between various parameters involved in the steam explosion pretreatment process have been modeled—both those related to biomass composition and process-specific variables—with the goal of optimizing the final composition of the resulting product.

In this project, several multilayer perceptron networks will be developed using the same initial dataset, and their outputs will later be ensembled using the bootstrap method (García Fernández et al., 2025) to enhance the reliability of the results (Berzal, 2018).

The multilayer perceptron (Figure 1) can be described as a computational system that mimics the computational abilities of biological systems by employing a large number of interconnected elements. Its function-approximating capability (Hornik, 1989) allows it to model complex nonlinear relationships by extracting knowledge from a set of examples, which can then be applied to new, unknown situations.
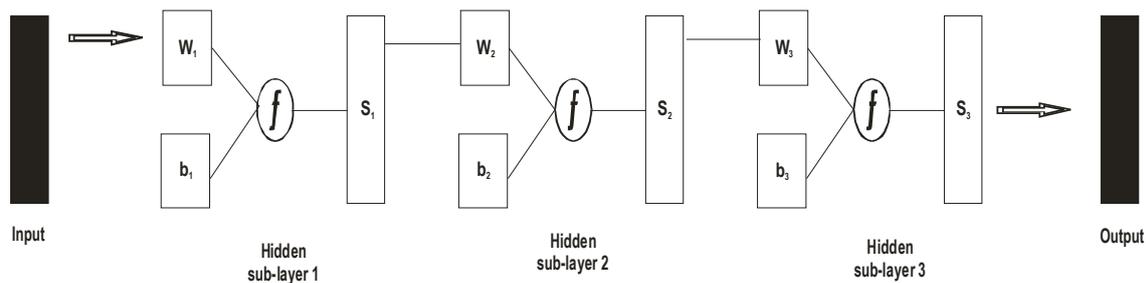
Figure 1. Feed-forward multilayer perceptron neural network

An MLP consists of three main layers: the input layer, the hidden layer(s), and the output layer. The input layer receives signals from the input variables and transmits them to the hidden layer. The hidden layer, which may include one or more sublayers, performs the mathematical operations required to generate the final output. The output layer presents the results computed by the hidden layer(s).

Designing a multilayer perceptron is a complex and time-consuming task. The number of neurons in the input layer is determined by the dimensionality of the input vectors, and the output layer size is defined by the output vector's dimension. However, there is no established rule for determining the number of hidden layers or the number of neurons in each. Consequently, the configuration of the hidden layer must be done through trial and error (Lin and Tseng, 2000). Some guidelines exist to ensure the convergence of the solution by optimizing internal parameters based on the size of the dataset (Lawrence et al., 1996; Sha, 2007; Xu, 2007). It is also important to note that an insufficient number of neurons in the hidden layers may lead to poor generalization, while an excessive number may hinder the learning process without significantly improving the final results (Cheng, 1995).

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Additionally, certain conditions must be met to ensure the neural network functions effectively, among which is the need to avoid overfitting, which severely limits the network's generalization ability (Bishop, 1995).

To prevent overfitting and estimate the network's reliability, the initial dataset was randomly divided into three subsets: training set (70% of the data), validation set (15%), and test set (15%). The training and validation sets were used during the training phase to guide learning and prevent overfitting, respectively. The test set was used to evaluate the final reliability of the model (Bishop, 1995).

Based on previous studies on this type of board (García Fernández et al., 2008; Esteban et al., 2009), in modeling internal bond, modulus of rupture, and modulus of elasticity, the input variables included panel thickness, density, moisture content at testing, swelling, and two-hour water absorption.

The chosen transfer function was the hyperbolic tangent sigmoid function (Eq. 1), which is mathematically equivalent to the hyperbolic tangent but improves the network's performance (Demuth et al., 2002).

$$f(x) = \frac{2}{1 + e^{(-2x)}} - 1$$

f(x).- Neuron output value.

x.- Neuron input value.

(1)

All input and output variables were normalized to enhance the efficiency of the transfer function (Eq. 2) (Demuth et al., 2002). The resilient backpropagation algorithm was used for training, as it provides superior results for sigmoid transfer functions (Demuth et al., 2002).

$$X' = \frac{X - X_m}{s}$$

X': Value after normalization of vector X.

X_m: Mean of vector X.

(2)

S: Standard deviation of vector X.

As a preliminary step in network design, a principal component analysis (PCA) was conducted on the input vector to identify correlations between variables and improve the network's performance (Demuth et al., 2002). Variables were selected based on their contribution exceeding 2% of the dataset's variability (Sarle, 1997; Demuth et al., 2002).[1–16]

3.2. Artificial Neural Networks Modelling in steam explosion pre-treatment (related to UPM→Latitud secondment)

Different types of biomass were used for the study: sugarcane bagasse, switchgrass, *Eucalyptus globulus*, pine sawmill residues, *Eucalyptus grandis*, *Arundo donax*, and pine. Their chemical composition was determined, including ash, water and ethanol extractives, soluble lignin and insoluble lignin, glucan, arabinan, xylan, galactan, and acetyl groups. The pretreatment conditions ranged between 170 and 200 °C and from 5 to 20 minutes.

The output of the steam explosion pretreatment (cellulose, hemicellulose, and lignin contents) was modeled based on the initial composition of the biomass (Ash, Water and ethanol extractives, soluble lignin and insoluble lignin, glucan, arabinan, xylan, galactan, and acetyl groups), and the process parameters of temperature and time.

The resulting networks showed high coefficients of determination:

- Cellulose: R^2 = 0.84
- Hemicellulose: R^2 = 0.90
- Lignin: R^2 = 0.76

These values indicate that the models are capable of explaining over 75% of the sample variability.

The process optimization aimed to find the most suitable temperature–time combination for a given chemical composition of biomass, in order to maximize the yield of either cellulose, hemicellulose, or lignin.

Starting from the following initial composition:

- Ash: 1.31
- H_2O + EtOH extract: 5.65
- Soluble lignin: 2.05
- Insoluble lignin: 18.14
- Glucan: 36.5
- C5 sugars: 20.15
- Acetyl groups: 5.5

The resulting optimization surfaces (Figures 2-4) reveal that higher temperature and longer pretreatment time lead to increased yields of cellulose and lignin (Figures 2 and 4), while hemicellulose content peaks at lower temperatures and shorter processing times (Figure 3).

In this particular case, the highest cellulose yield was obtained at 200 °C and 20 minutes, although significant production was also observed at 180 °C with treatment times between 10 and 20 minutes. However, the results indicate that the cellulose content was slightly lower under these conditions.

For hemicellulose, the opposite trend was observed: the highest yield was obtained under pretreatment conditions of 170 °C and 5 minutes.

In the case of lignin, the greatest production was achieved with a pretreatment of 200 °C for 20 minutes.
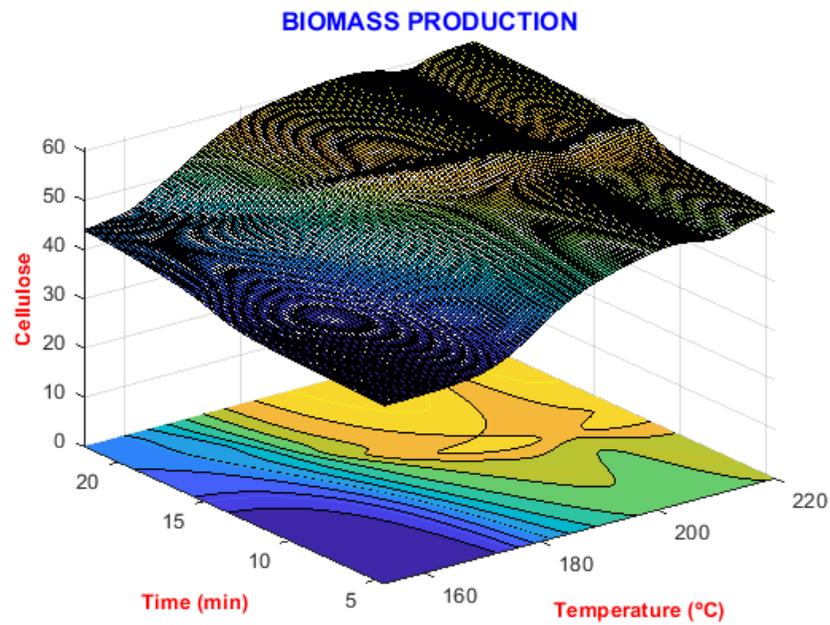
Figure 2. Optimization surface for cellulose production
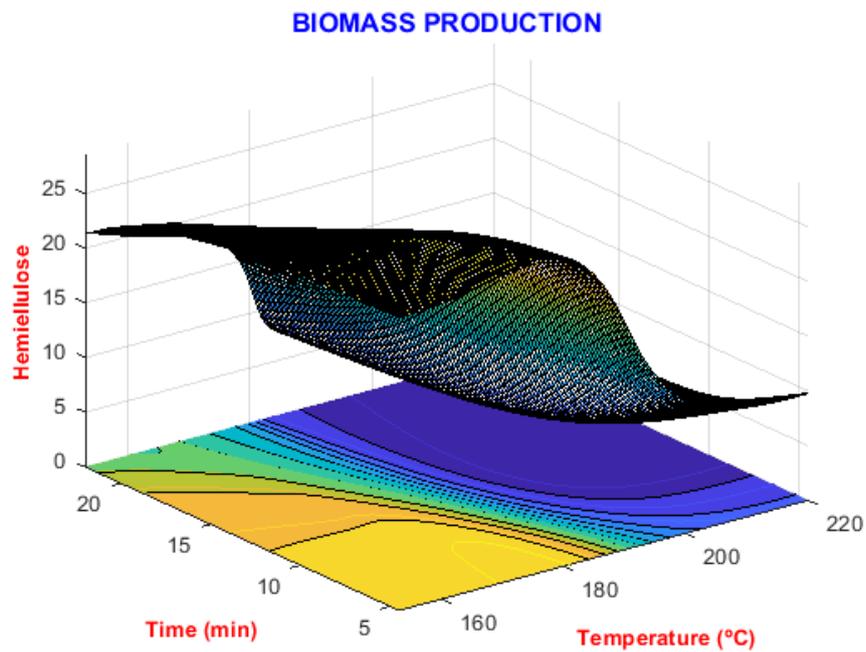
Figure 3. Optimization surface for hemicellulose production
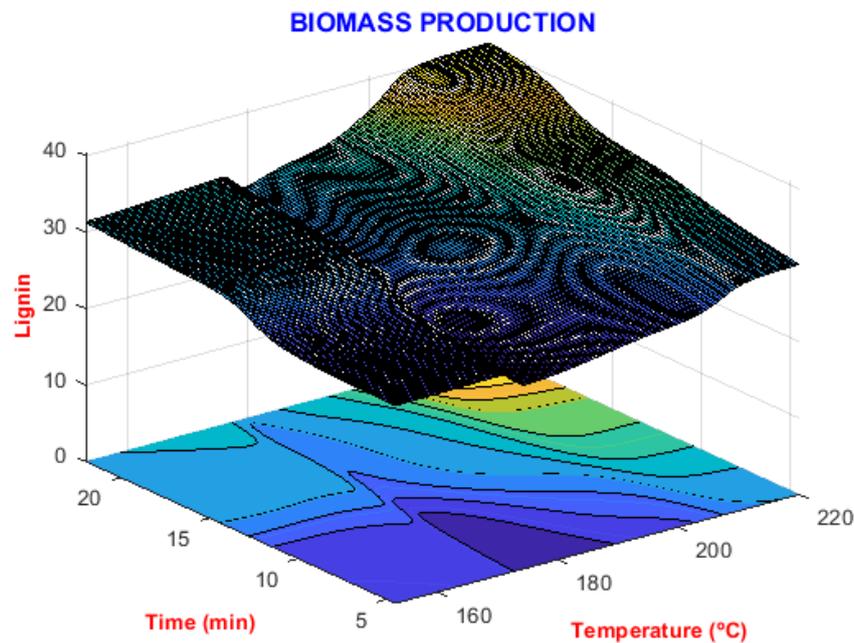
Figure 4. Optimization surface for lignin production

Conclusions:

- A mathematical simulator of the steam explosion process has been developed.
- Process parameters can be adjusted to evaluate system performance.
- Temperature and time can be optimized according to the desired product outcome.

3.3. Artificial Neural Networks Modelling in hydrothermal pre-treatment (related to UPM→ECORESOURCES secondment)

The biomass used for the experiment of this section were the commercially available beechwood sawdust (used as reference), olive tree prunings, vineyard prunings and peach kernels. Complete composition analysis was performed to determine the structural carbohydrates (glucan, arabinan, xylan, galactan, mannan and acetyl groups), the soluble lignin and insoluble lignin and the ash content. The pretreatment of biomass was carried out via hydrothermal/dilute acid pretreatment under autogenous pressure and the conditions ranged between 170-220°C, 15-180 minutes and 0-0.25 wt.% H_2SO_4.

The hydrothermal pretreatment was modeled for both the solid and liquid fractions, using the initial biomass composition (Ash, Water and ethanol extractives, soluble and insoluble lignin, glucan, arabinan, xylan, galactan, acetyl groups) and process parameters (temperature and time).

The same modeling methodology (as for steam explosion-5.2) was applied. However, due to the limited availability of primary data, the initial dataset was augmented using the Bootstrap simulation method.

For the final simulation, the starting composition was:

- Ash: 3.8
- Glucan: 22.85
- Xylan: 11.25
- Galactan: 0.75
- Arabinan: 4.56
- Mannan: 1.1
- Acetyl Units: 6.0
- Soluble lignin: 5.84
- Insoluble lignin: 34
- Extractives: 26.5
- H_2SO_4: None

The model was used to simulate the glucan content after pretreatment. Figure 5 shows the distribution of the predicted values, and Figure 6 displays the optimization surface for glucan recovery. As seen, optimal glucan output is achieved at lower pretreatment durations and temperatures close to 150°C .

In this study, the maximum glucan yield corresponded to a pretreatment temperature of 150 °C and a reaction time of 15 minutes.
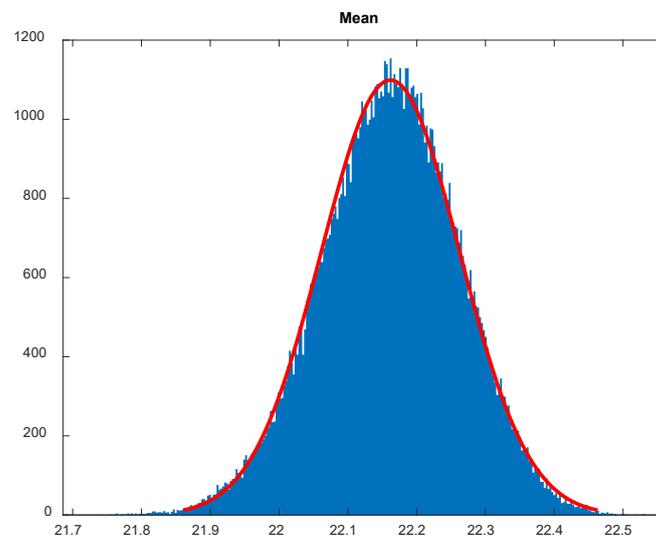
Figure 5. Distribution of the obtained value (Glucan: 22.16%)
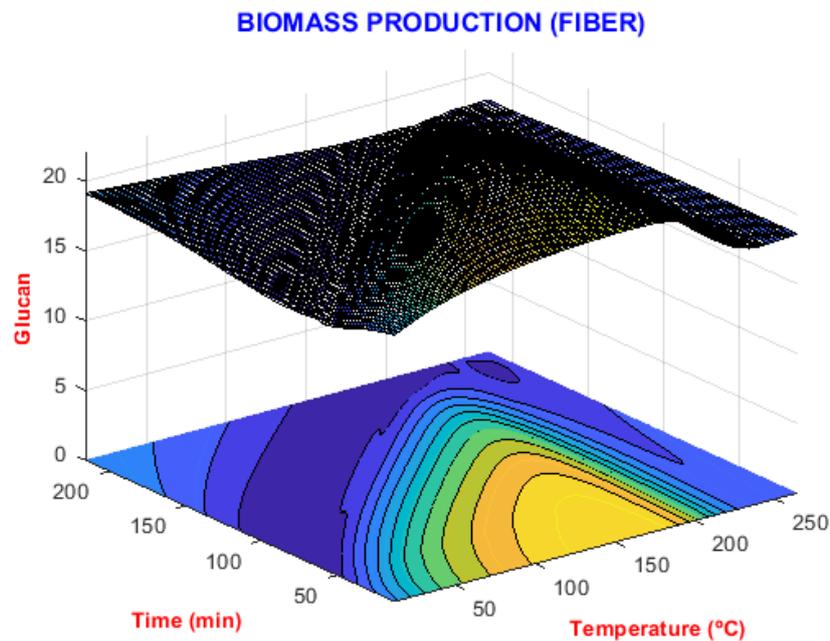
Figure 6. Optimization surface for glucan production

Conclusions:

- A mathematical simulator of the steam explosion process has been developed.
- Process parameters can be adjusted to evaluate system performance.
- The distribution function of the value simulated by the neural network has also been obtained.
- Temperature and time can be optimized according to the desired product outcome.

4. PART B – SIMULATION AND OPTIMISATION (TASK 2.2)

4.1. Introduction to process modelling and techno-economic analysis

Process modelling (simulation) is an essential tool in modern chemical engineering, enabling researchers and engineers to design, evaluate, and optimize chemical processes before they are implemented at scale. By using mathematical representations of unit operations (reactors, distillation columns, heat exchangers, separation systems etc.) process modelling provides a means to predict mass and energy flows, product yields, and process efficiencies. Software packages, including Aspen Plus, DWSIM and others, allow the integration of thermodynamics, kinetics, and transport phenomena into simulations that mirror real-world chemical plants reducing experimental costs, and providing insights into process feasibility and potential bottlenecks.

While process modelling focuses on technical performance, it is equally important to assess the economic viability of a process. Techno-economic analysis (TEA) combines modelling with financial evaluation, linking process design to capital investment, operating costs, and expected revenues helping to assess the viability of a potential investment in a specific process or production. This dual perspective ensures that innovations are not only technically sound but also competitive in the marketplace.

The report gives a review of the process modelling and TEAs that have been done using input from WP1 under CELISE project during the various secondments and/or internal research of the parties.

Specifically, **6 cases are reported as shown below:**

Case 1: Process modelling of barley's spent grain to bioethanol

Case 2: Process modelling of Algae (*Ulva rigida*) to different valorisation options

Case 3: Feasibility study of lignocellulosic loose-fill thermal insulation material using steam explosion technology

Case 4: Techno-economic analysis of the production of phenolic and furanic fractions/compounds from biomass.

Case 5: Techno-economic analysis of Kraft lignin fast (catalytic) pyrolysis for the production of high value-added chemicals (HVACs)

Case 6: Process modelling of chitosan production from dead bees

4.2. Case 1: Process modelling of barley's spent grain to bioethanol (related to UC to FICH-UNL and FICH-UNL to UC secondments)

This repor is focused on the valorisation of Brewers' Spent Grain (BSG). BSG is the main solid by-product of the brewing industry, representing about 85% of its residues. Rich in cellulose, hemicellulose, lignin, proteins, and starch, BSG is a promising feedstock for sustainable bio-based processes. The first step was to investigate the dilute acid hydrolysis of BSG to obtain sugar-rich streams. The second one extends this concept towards the production of second-generation (2G) bioethanol through a process chain combining acid hydrolysis, enzymatic hydrolysis, fermentation, and purification.

Brewing Industry and BSG

Europe is the second largest beer producer worldwide. In Spain, production exceeded 41 million hectolitres in 2022, consolidating it as the second EU producer after Germany. The industry generates several residues, among which BSG is predominant. Depending on the production scale, BSG is either used as animal feed, discarded, or occasionally valorised. Its annual global production is estimated at 39–40 Mt, offering a low-cost, year-round available biomass source.

Figure 7 shows the process of the brewery.
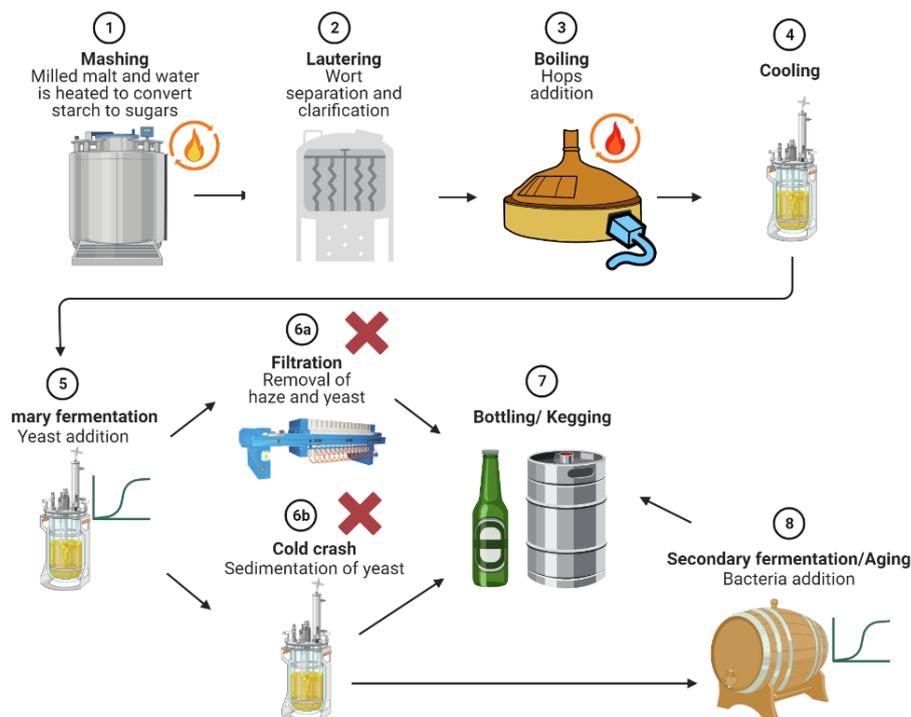
Figure 7. Overview of the brewing process (Ramanan et al., 2024[17])

Composition and Characteristics of BSG

BSG is mainly composed of cellulose (~20%), hemicellulose (~17–31%), lignin (~20–28%), proteins (~20–25%), and variable amounts of starch (1–7%). This composition depends on barley type, agronomic conditions, and brewing processes. The polysaccharide fractions provide

fermentable sugars after hydrolysis, while proteins and phenolic compounds can add value in other sectors. However, high moisture (~70–80%) and heterogeneity limit its direct use.

Methodologies

Both studies applied a combined methodological approach:

- Physicochemical characterisation of BSG (humidity, polysaccharides, lignin, starch).
- Dilute acid hydrolysis experiments at different temperatures (90°C, 100°C, 120°C).
- Kinetic modelling of hydrolysis reactions to predict sugar release.
- Simulation of 2G bioethanol production using Aspen Plus.

Results

The experiments demonstrated that dilute acid hydrolysis effectively liberates fermentable sugars. Figure 8 shows the kinetic results. At 120°C, hydrolysis achieved 62.4% conversion of glucan to glucose and 41% conversion of xylan/arabinans to xylose/arabinose. Kinetic models matched experimental data, confirming the process reliability.
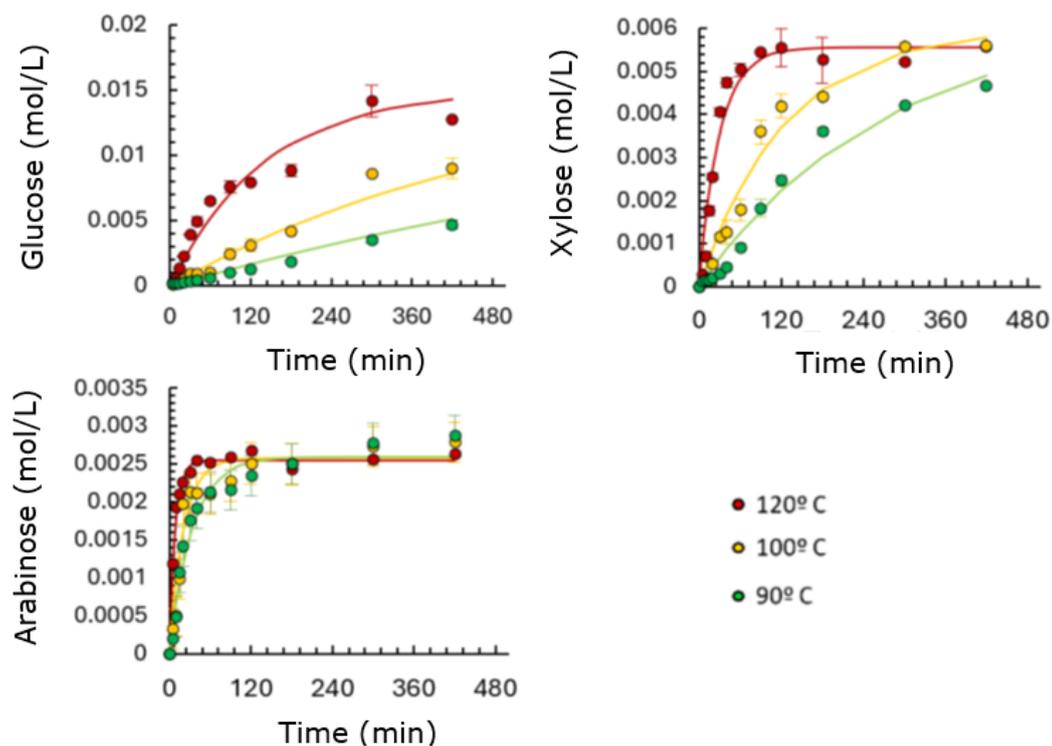
Figure 8. Kinetic results of BSG

Aspen Plus simulations estimated that 110 kg/day of wet BSG (≈24 kg dry) could produce 6.49 kg/day of ethanol at 99.95% purity. While promising, this yield is modest, highlighting the need for residue unification across multiple breweries to ensure industrial viability. Figure 9 shows the simulation process.
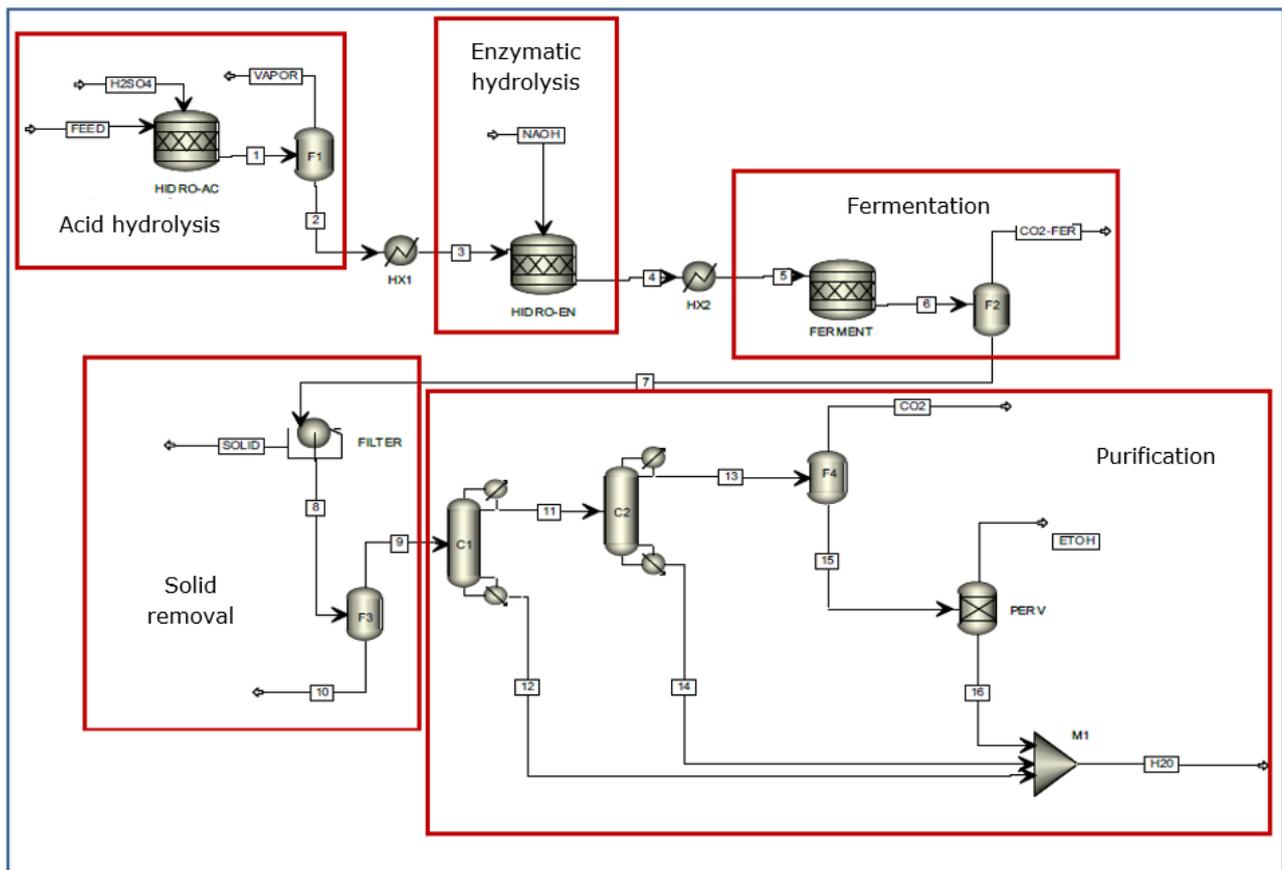
Figure 9. Simulation of bioethanol from BSG with Aspen.

Conclusions

Both theses demonstrate the potential of BSG valorisation within a circular bioeconomy framework. Dilute acid hydrolysis provides a reliable method to obtain fermentable sugars, which can then be converted into 2G bioethanol. Despite the relatively low yields at artisanal scale, scaling up and combining resources across breweries could improve feasibility. Beyond biofuels, BSG also offers opportunities in food, materials, and chemical industries.

4.3. Case 2: Process modelling of Algae (*Ulva rigida*) to different valorisation options (related to FICH-UNL to UC secondments)

This report is focused on the valorisation of *Ulva rigida*, a green macroalga, as feedstock for 3rd generation biorefineries. The first case analyses the potential of Ulva residues for bioethanol production through acid hydrolysis, fermentation, and techno-economic evaluation. The second one extends the approach to the production of biobutanol via the Acetone-Butanol-Ethanol (ABE) fermentation pathway, supported by Aspen Plus modelling.

Background: Macroalgae as Feedstock

Global macroalgae production reached nearly 33 million tonnes in 2017, dominated by anthropogenic cultivation in Asia. Macroalgae are classified into brown, red, and green types, each with characteristic polysaccharides. Ulva rigida, the selected green macroalga, contains significant amounts of ulvan, cellul_____ it a promising biomass for sustainable fuels and chemicals.

Methodologies

Both cases combined experimental characterisation of Ulva rigida with process simulation:

- Experimental analyses: grinding and sieving, moisture and ash content, extractives, cellulose, hemicellulose, holocellulose, and sugar profiling (HPLC).Process modelling in Aspen Plus: hydrolysis, fermentation, and purification stages.
- The first one is for bioethanol process modelling and techno-economic analysis.
- The second one to biobutanol via ABE fermentation, including validation of hydrolysis and fermentation steps.

Results

Experimental results showed Ulva rigida has ~93% moisture, ~18% ash, ~10% cellulose, and ~18% hemicellulose. Detected sugars include rhamnose, glucose, xylose, and uronic acids. Gallart (2021) demonstrated the feasibility of two-step hydrolysis releasing fermentable sugars, with simulated ethanol production supported by techno-economic modelling.

It was obtained simulated production of ~2666 kg/h of butanol, 678 kg/h acetone, and 41 kg/h ethanol from 50,000 kg/h of dry Ulva rigida, with product purities above 82–99%. The hydrolysis stage was the most energy- and cost-intensive. Capital investment was estimated at ~€13M, with operating costs of ~€59M.

Figures 10 and 11 show the diagrams of the processes.

Figure 10. Simualtion of Ulva rigida biorefinery process for obtaining ABE

Figure 11. Simualtion of Ulva rigida biorefinery process for obtaining bioethanol

Conclusions

The integrated findings show that Ulva rigida is a promising feedstock for 3rd generation biofuels, providing fermentable sugars and polysaccharides for conversion into ethanol and butanol. Techno-economic analysis indicates that process viability strongly depends on scaling and integration with other products (e.g., ulvan extraction) to offset high hydrolysis costs. Both theses underline the potential role of macroalgae-based biorefineries in future sustainable energy strategies.

4.4. Case 3: Feasibility study of lignocellulosic loose-fill thermal insulation material using steam explosion technology

The **purpose** of the feasibility "Commercialization of lignocellulosic loose-fill thermal insulation material production technology" was to assess and analyze the introduction of a potentially new product (lignocellulosic loose-fill thermal insulation material) and a potentially new technology (lignocellulosic loose-fill thermal insulation technology by the steam explosion method) in order to objectively and rationally identify the advantages, disadvantages, opportunities and threats of the new product and technology, as well as identify the resources needed and the prospects for implementation of commercialization.

The **tasks** of the feasibility study were following:

1) To perform an analysis of the new product;
2) To perform an analysis of the analogue products market and potential sales markets;
3) To analyze intellectual property rights protection measures;

4) To analyze the current and planned cooperation with other research organizations and businesses;
5) To perform a cost-benefit analysis of product commercialization.

The feasibility study has been conducted in accordance with definition of Article 2 (87) of Regulation (EU) No 651/2014, as well as in accordance with Implementing rules for the measure 1.2.1.2 "Support for the improvement of the technology transfer system" of specific support measure 1.2.1 "Increasing private sector investments in R&D" of the Cabinet Regulation No. 692 "Operational Program "Growth and Employment" of 25.10.2016.

The potentially new product and its technology analysed in the document **correspond to two areas of RIS3 specialization** - Smart Materials, Technologies and Engineering Systems and the Knowledge-intensive Bioeconomy. Thus, the research of lignocellulosic loose-fill thermal insulation material production technology is interdisciplinary. The introduction of lignocellulosic loose-fill thermal insulation material in production in sectors of the Latvian economy with high added value will promote the increase of the international competitiveness of Latvian companies and their penetration into new foreign markets. However, LSIWC will consider the possibility of commercializing the new product and technology in European and global markets as well.

The product and technology have a high level of innovation – thermal insulation material obtained by steam explosion technology is not currently available on the market. The high innovation aspect of the product is confirmed by the obtained Latvian patent No EN 15328 (see Annex No. 1) and scientific articles developed by the project team (see Annex No. 2). The results of previous research by LSIWC will be used in the commercialization of the product.

Currently, the product has been developed and validated in an artificial (laboratory) environment up to TRL4. LSIWC has obtained samples of thermal insulation material in small quantities under laboratory conditions using a 0.5L steam explosion device. In Phase 2 of the Project, it is planned to develop the product up to the TRL6. In Phase 2 of the Project, pilot batches of thermal insulation material will be produced, testing the technology at the level of the pilot plant and verifying the properties of the product in a real operating environment (wooden frame houses).

305,510.43 euros are needed to bring the product to be commercialized from the current TRL4 to the commercial TRL6. It is planned to attract funds using ERDF co-financing under the measure 1.2.1.2 "Support for the improvement of the technology transfer system" and other public funding (LSIWC core funding). In the Phase 2 of the Project, it is planned to implement **only such activities that are not of an economic nature.**

At least 5 current LSIWC employees will be involved in Phase 2 of the Project:

- Scientific supervisor of the project Dr.sc.ing. Ramunas Tupciauskas, who is the co-author of patent LV 15328 (see Annex No. 1) and co-author of several scientific publications on the topic of the project (for scientific publications, see Annex No. 2). Has supervised the development of contract research for industry partners. Ramunas Tupciauskas has been working as a researcher at LSIWC since May 11, 2012, but since July 22, 2020 he has been elected as a leading researcher.

- Commercialization expert Mg.sc.ing. Martins Andzs, who is the co-author of the patent LV 15328 and co-author of many scientific publications on the project topic (for scientific publications, see Annex No. 2). An experienced entrepreneur with practical experience in the commercialization of new products and technologies.

- Financial analyst and project administrative manager Mg.oec. Karina Orlova with 10 years of experience in management, commercialization and entrepreneurship of projects financed by the EU structural funds. She has supervised managed and EU structural funds

co-financed projects in both scientific institutions and private companies. Specializes in science project and production infrastructure project management.

- Two scientific assistants.

The project corresponds to the direction of national economy transformation "Sectors of future growth, where high value-added products and services exist or may arise", Priority 2 "Constant search for new products/services, within which it is necessary to create an effective identification system capable of finding and providing support to create new products within existing and cross-sectoral sectors, as well as to create new sectors with high growth potential".

As a result of the feasibility study, **it was concluded** that lignocellulosic lose-fill thermal insulation material is a **product with a high commercialization potential**. The product is made from renewable natural resources and production by-products that is safe for human health. There are no significant barriers to the commercialization of the product. The product to be commercialized **can play an important role in expanding fast-growing markets, due to which it has a particularly high investment potential**.

More information can be found here

4.5. Case 4: Techno-economic analysis of the production of phenolic and furanic fractions/compounds from biomass.

Introduction

An evaluation of the economic parameters of the production of phenolic and furanic fractions/compounds from biomass was carried out. Residues from agricultural activities, as well as waste from related agricultural and food processing industries, were used as a ligno-cellulosic biomass feedstock. This was an external funded project, by EU and Greek National Funds, conducted with the collaboration of AUTH and Chimar S.A.

The isolation of hemicellulose and lignin was carried out through hydrothermal pretreatment in batch reactors, with dissolved water and dilute acid solution, at 170°C for 15 minutes. From this treatment, a liquid fraction rich in semi-cellulose and a solid fraction consisting of cellulose and lignin are obtained. At a later stage, cellulose is hydrolyzed in the presence of enzymes to produce glucose, while lignin remains as a solid residue (hydrolysis lignin). Alternatively, the Organosolv method was studied as a pretreatment and fractionation method, in which hydrothermal treatment is carried out in an ethanol/water mixture aiming at the simultaneous removal of hemicellulose and lignin in one stage. Subsequently, lignin undergoes rapid pyrolysis for the production of biooil which contains mainly alkoxy and alkyl-phenolic compounds, while by catalytic acid hydrolysis/dehydration processes, the hemicellulose sugars (mainly xylan/xylose) are converted into furanic compounds (mainly furfural) and organic acids.

In the context of the study, the results of the techno-economic evaluation for the production of (1 kg) of lignin and furfural from 2 types of biomass pre-processing (Organosolv and Hydrothermic) are presented, as well as the cost of production (1 kg) of bio-oil from lignin pyrolysis.

The design of the 3 industrial production units of the above products (Organosolv pretreatment, hydrothermal pretreatment, lignin pyrolysis) was carried out. The study has been performed according to the methodology by Peters and Timmerhaus[18]

Operational data

The operational parameters are given in Tables 1-3.

Table 1. Operational Parameters of Biomass Pretreatment Plants - Organosolv

	Production stages		
	Organosolv pretreatment	Enzymatic hydrolysis	Acid hydrolysis
Batchtime (h)	3	74	3
Main product	Organosolv lignin	Enzymatic hydrolysis lignin	Furfural
Batches per year	2448	99	2448
Production rate (tonne/yr)	252.28	275.22	31.87

Table 2. Operational Parameters of Biomass Pretreatment Plants - Hydrothermal

	Production stages		
	Hydrothermal pretreatment	Enzymatic hydrolysis	Acid hydrolysis
Batchtime (h)	3	74	3
Main product	Acid soluble lignin	Enzymatic hydrolysis lignin	Furfural
Batches per year	2448	99	2448
Production rate (tonne/yr)	170.90	722.13	231.93

Table 3. Operational Parameters of Lignin Pyrolysis Plant

	Lignin pyrolysis
Batch time (h)	2
Main product	bio-oil
Batches per yr	3672
Production rate (tonne/yr)	418.61

Table 4 shows the experimental input data used for the individual processes, which resulted from inhouse studies.

Table 4. Experimental data - Input, reactants

	Hydrothermal pretreatment	Organosolv Pretreatment	Lignin Pyrolysis
Biomass (g)	60	30	-
H_2O (g)	300	120 (+700)	-
H_2SO_4 (g)	1.37	0.587	-
Ethanol (ml)	-	180	-
Lignin (g)	-	-	0.505
Silica Sand (g)	-	-	0.501
Phenol (g)	-	-	-
Formaldehyde (37 wt.%) (g)	-	-	-
NaOH (g)	-	-	-
Bio-oil (g)	-	-	-
Furfural (g)	-	-	-

The prices of raw materials, utilities and labor are given in Table 5

Table 5. Cost of raw materials/utilities/labor

	cost	unit
Biomass	0.08	EUR/kg
H_2SO_4	0.28	EUR/kg
Furfural (commercial)	1.20	EUR/kg
Ethanol	1.44	EUR/kg
Cellulase	5.00	EUR/kg
N_2	0.03	EUR/kg
Water (distilled)	0.004	EUR/kg
Electric energy	200	EUR/MWh
Natural gas	200	EUR/MWh
Cooling water	0.005	EUR/kg
Labor	12	EUR/person/h

Results

Flowcharts

Figure 12 shows the flowchart for the hydrothermal pretreatment.
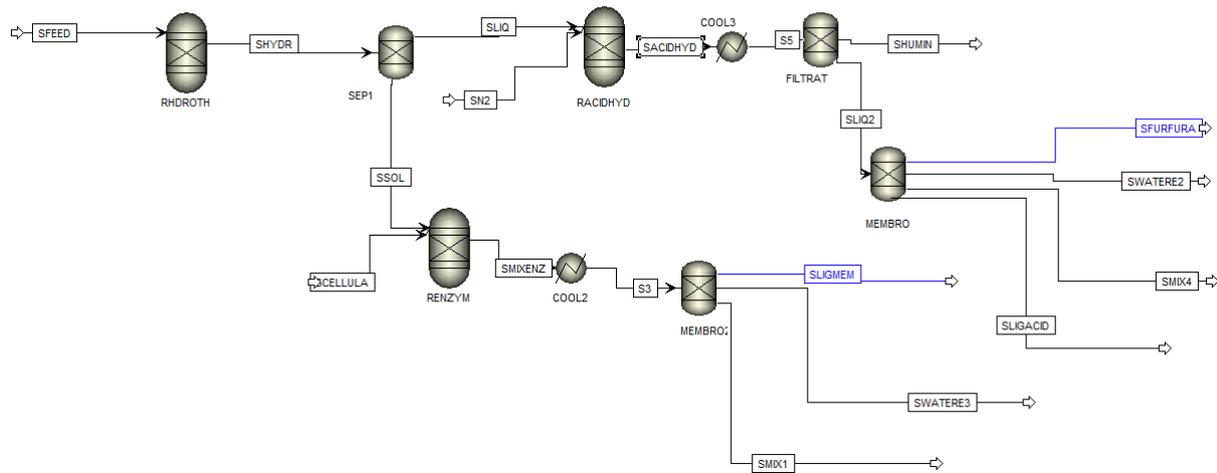
Figure 12. Flowchart – Hydrothermal pretreatment

Figure 13 shows the flowchart for the hydrothermal pretreatment.
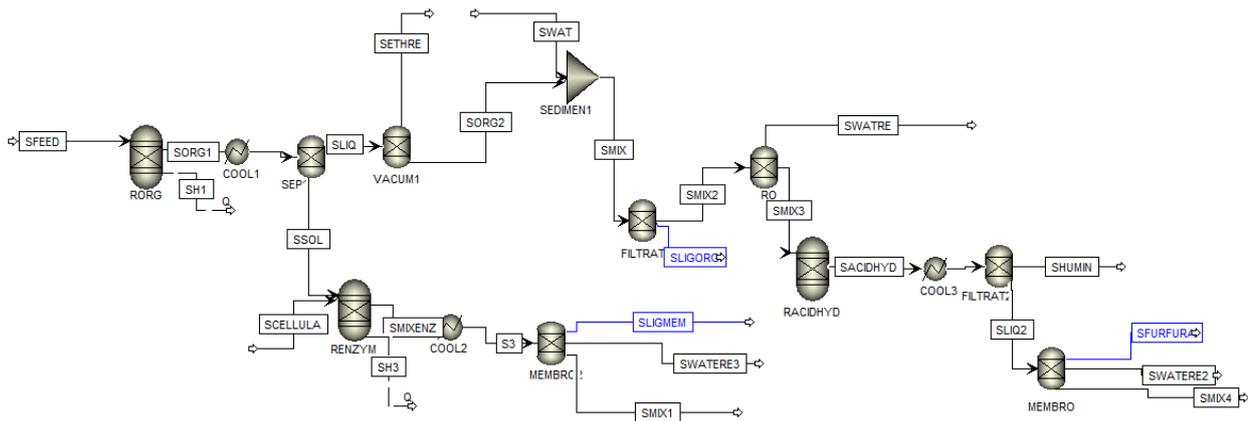
Figure 13. Flowchart – Organosolv pretreatment

Figure 14 shows the flowchart for the lignin pyrolysis.
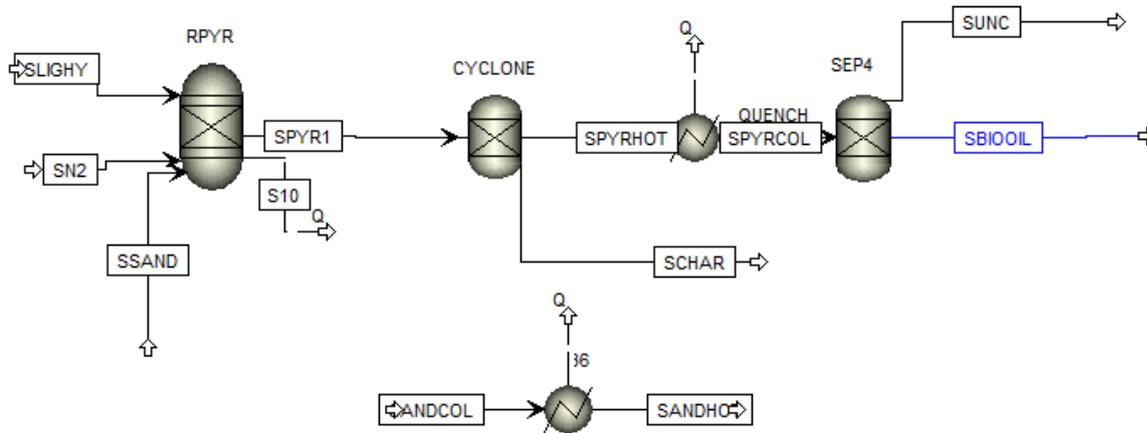
Figure 14. Flowchart – Lignin pyrolysis

CAPEX/OPEX

Table 6 shows the details of the equipment as well as the total purchase cost and Table 7 shows the main production costs.

Table 6. Aggregated equipment data

Equipement	Hydrothermal pretreatment	Organosolv pretreatment	Lignin pyrolysis
Reactors (pc)	4	3	1
Biomass Loading (pc)	1	1	-
Pump (pc)	7	8	2
Mixing/separation (pc)	4	7	2
Storing tank (pc)	6	6	1
Heat exchanger (pc)	3	3	1
Purchase cost (EUR)	**195000**	**225000**	**115000**

*Press

Table 7. Annual main production costs

	Hydrothermal pretreatment	Organosolv pretreatment	Lignin pyrolysis
Raw materials (EUR/yr)	860,545.208	1,851,365.11	296,697.60
Utilities (EUR/yr)	462,527.50	418,710.85	11,383.20

Direct labor (EUR/yr)	1,121,280.00	1,121,280.00	280,320.00
Waste management	0.00	0.00	0.00

Figure 15 shows the CAPEX for all cases.
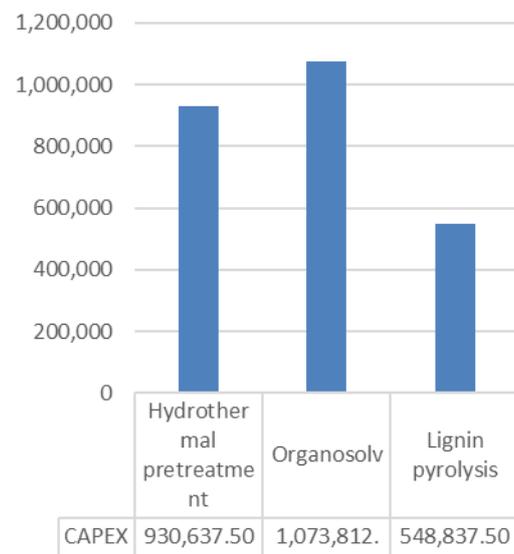
Figure 15. Capex for all cases

Table 8 shows the production costs for Organosolv and hydrothermal pretreatment

Table 8. Production costs for Organosolv and hydrothermal pretreatment

	Products with organosolv pretreatment		Products with hydrothermal pretreatment		
	Annual production (kg ή m³ for boards)	Production cost	Annual production (kg ή m³ for boards)	Production cost	unit
Enzymatic hydrolysis lignin	286285.48	6.37	722131.66	3.99	EUR/kg
Organosolv lignin (or acid soluble for hydrothermal pretreatment)	252282.98	2.96	170902.4514	0.04	EUR/kg
Furfural	44691.04	0.53	231930.75	0.06	EUR/kg
Mix 1	620500.09	0.00	722244.13	0.00	EUR/kg
Mix 4	132558.76	0.00	687938.46	0.00	EUR/kg
Humins	16348.28	0.00	1137348.32	0.00	EUR/kg
Bio-oil	418608.00	11.79	418608.00	8.64	EUR/kg

* Panel dimensions: 1,20m x 2,40m x 0,3mm

Conclusions

The results of the study show that the hydrothermal pretreatment of lignocellulosic biomass is the most economical method in terms of both production and fixed capital costs (CAPEX). Specifically, the CAPEX for the hydrothermal pretreatment plant is approximately 16% lower than that with organosolv. The production cost of lignin biooil is much higher through the pyrolysis of Organosolv lignin compared to lignin isolated after hydrothermal pretreatment of the biomass. The production cost of furfural is significantly lower compared to lignin biooil. Mix 1, Mix 4 and humines have been treated as products for sale at zero cost. If treated as waste, the parameters of production costs will change for all processes as waste management costs will be added.

4.6. Case 5: Techno-economic analysis of Kraft lignin fast (catalytic) pyrolysis for the production of high value-added chemicals (HVACs) (related to AUTH→CCC secondment)

Introduction

Six distinct scenarios of innovative industrial-level plants that use fast pyrolysis to valorise kraft lignin are screened in this research (detailed in the following section). Modelling the process, using a fluidised bed reactor, scenarios 1 and 2 are utilised as the base case to evaluate the economic parameters of thermal fast pyrolysis (TFP) and catalytic fast pyrolysis (CFP), with electric energy serving as the primary source of income. The primary source of income, high value-added chemicals (HVACs), are provided by a separation section in scenarios three through six. For every scenario, a techno-economic analysis—a method for evaluating an industrial plant's financial performance—has been carried out. This study aims to compare the economic performance of six plants using lignin catalytic and thermal fast pyrolysis to produce high-value chemicals and energy. It does this by listing and evaluating a set of economic indicators for industrial-scale plants. The second goal is to evaluate the benefits and drawbacks of catalytic versus thermal rapid lignin pyrolysis for the generation of bio-based compounds and electrical energy. The third goal is to compare three different bio-oil separation techniques by providing simulation data.

Scenarios

Figure 16 shows a brief summary of the scenarios studied as mentioned in the introduction.
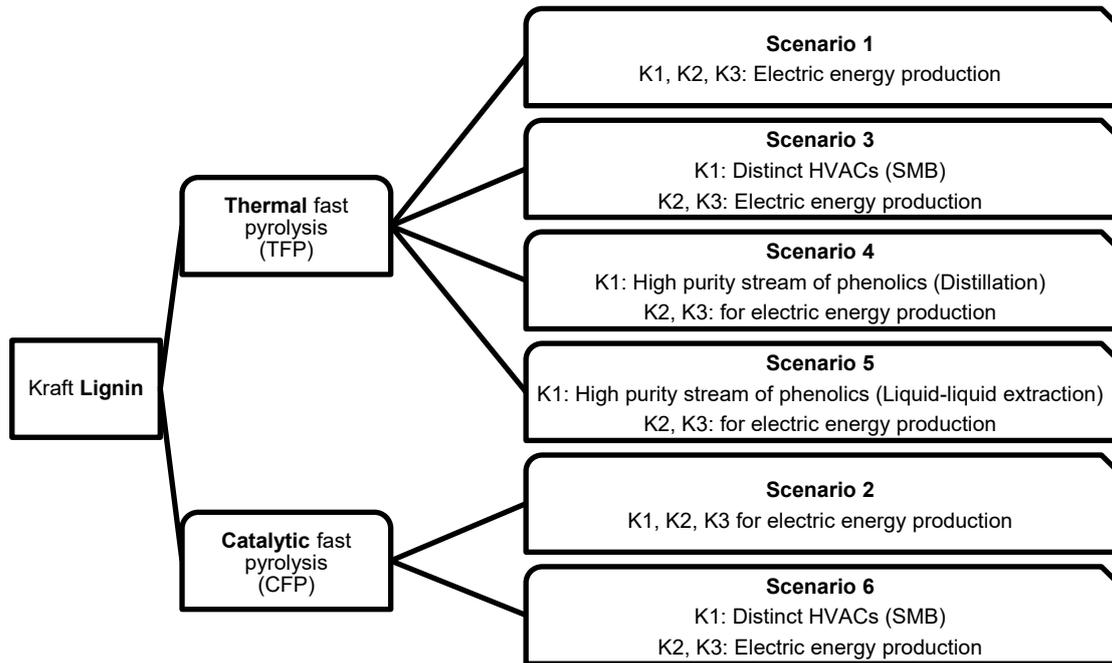
Figure 16. Overview of the studied lignin pyrolysis scenarios regarding bio-oil valorization

The processes have been modelled in Apsen plus with a descriptive (not the flowchars used) flowchart shown in Figure 17 while a detailed flowchart of the model is presented in Figure 18. The separation section is different for scenarios 3-6 and consists of Simulated Bed Chromatography-SMB for scenarios 3 and 6, distillation for scenario 4 and liquid-liquid extraction for scenario 5.
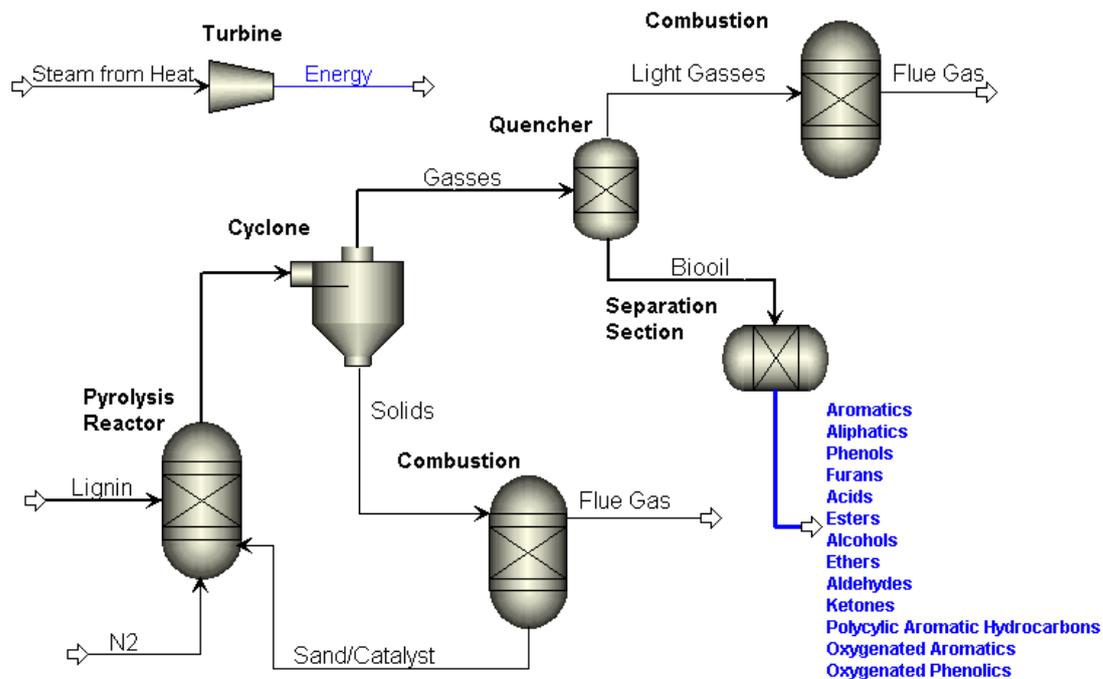
Figure 17. Simplified flowchart of the valorization process of kraft lignin pyrolysis towards the production of energy and HVACs
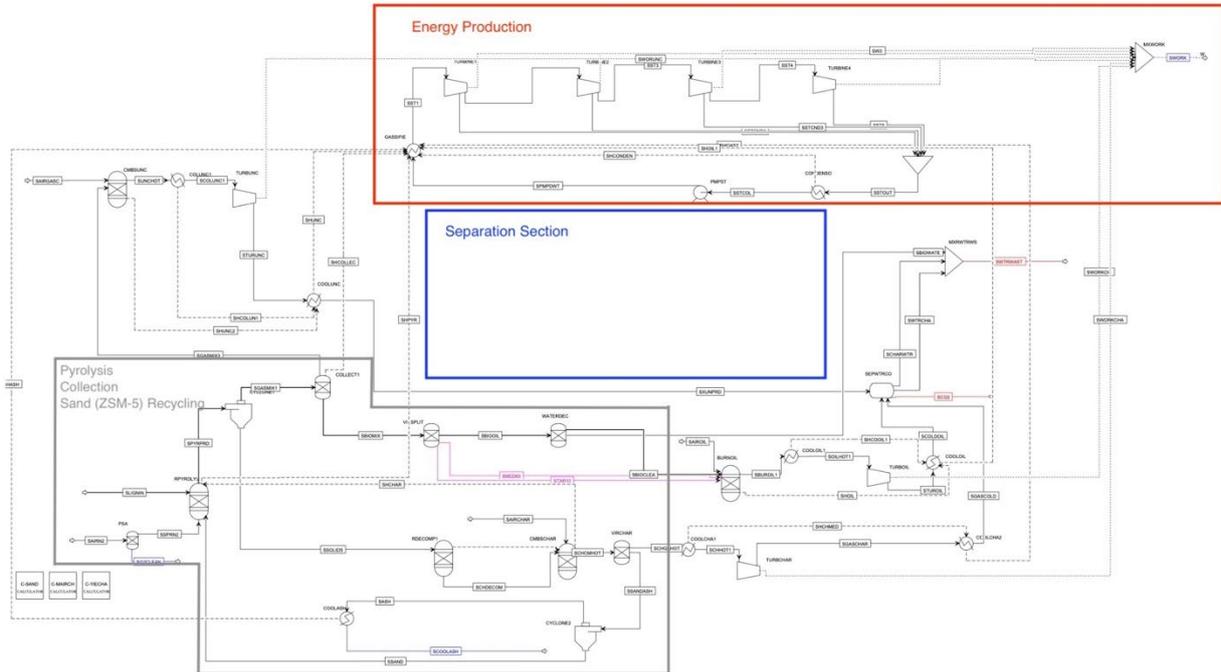
Figure 18 Detailed flowchart of the studied integrated process

The simulation input data, in terms of pyrolysis product yields, i.e. bio-oil, water (contained in bio-oil) non-condensable gases, solids (char and reaction coke), was retrieved from the work of Lazaridis et. al[19] and are given in summary on Tables 9-11.

Table 9. Product yields of kraft lignin thermal and catalytic (with ZSM-5 zeolite) pyrolysis

Products	Thermal (wt% on lignin)	ZSM-5 (wt% on lignin)
Bio-oil	32.94	16.80
Water	6.57	9.65
Gases	15.06	23.86
Char and coke	45.43	49.69

Table 10. Organic phase composition (relative concentration, GC-MS, % peak area) of bio-oil from kraft lignin thermal and catalytic pyrolysis

Contents	Thermal (% on GC-MS)	ZSM-5 (% on GC-MS)
Aromatics (AR)	0.10	37.23
Aliphatics (ALI)	0.00	6.08
Phenols (PH)	5.72	14.42
Furans (FUR)	0.62	0.00
Aldehydes (ALD)	0.29	0.00
Ketones (KET)	3.46	0.00
Polycyclic aromatic hydrocarbons (PAHs)	0.00	16.12
Oxygenated aromatics (OxyAR)	0.77	0.00
Oxygenated phenolics (OxyPH)	74.58	5.18
Unidentified (UN)+Sulfur (SUL)**	14.46	20.97

AR-Aromatics; ALI-Aliphatics; PH-Phenolics; FUR-Furans; ETH-Ethers; ALD-Aldehydes; KET-Ketones; PAHs: Polycyclic aromatic hydrocarbons; OxyAR-Oxygenated Aromatics; OxyPH-Oxygenated Phenolics; UN+SUL-Unidentified and Sulfur compounds.

** Not detected in GC-MS but entered for consistency reasons in the simulation.

Table 11. Composition of pyrolytic non-condensable gases

Compound	Kraft thermal (wt% on lignin)	Kraft ZSM-5 (wt% on lignin)
CO_2	6.89	9.23
CO	4.41	8.30
Methane	3.44	3.73
Ethane	0	0.31
Ethylene	0	1.45
Propane	0.32	0.21
Propylene	0	0.63

Techno-economic assessment framework

Equipment costing was performed in a consistent manner throughout the scenarios. However, determining the precise cost for equipment in low TRL projects is challenging[20]. Therefore, the results are meant to be used as a comparison between the different scenarios rather than as a real case investment data. The TEAs of this study have been performed using factors on top of

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the equipment purchase cost (PC) for the respective CAPEX parameters according to the methodology of Peters and Timmerhaus[18] and estimations.

Costing data

Table 12 shows the prices of raw materials, utilities and labor used in the study

Table 12. Prices of raw materials, utilities and labor used in the study.

	Type	price (EUR/unit)	unit
Kraft Lignin	Raw material	0.38	kg
Sand	Raw material	0.4	kg
ZSM-5	Raw material	5	kg
Ethyl acetate	Raw material	1.175	kg
Hexane	Raw material	10	kg
Diethyl Ether	Raw material	2.4	kg
NaOH	Raw material	0.3	kg
Labor	Labor	12	person/h
Electric Energy (purchase)	Utilities	0.0962	kWh
Cooling water	Utilities	0.00245	kg
Water Waste management	Utilities	0.036	kg
Water for steam	Utilities	0.00245	kg

Results

Table 13 gives the details of all the in and out streams as estimated by Aspen for the 6 scenarios of lignin pyrolysis products exploitation and the types of HVACs which can be recovered in each scenario are presented in Table 14. Scenarios 3 and 6 can give distinct chemical compounds in high purity by means of a simulated moving bed separation of the light fraction of bio-oil. In contrast, only mixtures of chemical groups can be recovered in scenarios 4 and 6. In scenario 4 a stream of 93.22% purity of oxygenated phenolics can be recovered while a stream of 92.88% purity can be recovered from scenario 5.

Table 13. In/out data for the 6 scenarios of kraft lignin pyrolysis towards the production of energy and HVACs.

	Type	Category	units	Scenario 1	Scenario 2	Scenario 3	Scenario 4	Scenario 5	Scenario 6
IN	Lignin	Raw Material	kg/h	6000	6000	6000	6000	6000	6000
	ZSM-5	Raw Material	kg/h	-	240	-	-	-	240
	Air	Raw Material	kg/h	53873.59	52873.59	49373.59	48373.59	48373.59	48873.59
	Ethyl Acetate	Raw Material	kg/h	-	-	20.22	-	-	20.22
	Hexane	Raw Material	kg/h	-	-	19.78	-	-	19.78
	Diethyl Ether	Raw Material	kg/h	-	-	-	-	49.20	-
	NaOH	Raw Material	kg/h	-	-	-	-	399.97	-
	HCl	Raw Material	kg/h	-	-	-	-	364.61	-
	Electric energy	Utilities	kWh	278.20	265.35	504.65	263.08	313.79	501.44
OUT	CO_2	Emissions/Waste	kg/h	14778.77	14785.28	13207.40	13207.40	13207.40	13797.95
	O_2	Emissions/Waste	kg/h	81.32	355.08	347.54	114.65	114.65	283.14
	NO_2	Emissions/Waste	kg/h	0.0019	0.0085	0.0083	0.0027	0.0027	0.0068
	NO	Emissions/Waste	kg/h	0.0664	0.1362	0.1293	0.0704	0.0704	0.1185
	CO	Emissions/Waste	kg/h	4.81E-07	2.30E-07	2.45E-07	4.06E-07	4.06E-07	2.23E-07
	N_2	Emissions/Waste	kg/h	41330.86	40564.57	37878.96	37111.90	37111.90	37496.25
	H_2	Emissions/Waste	kg/h	3.43E-08	1.25E-08	1.96E-08	2.93E-08	2.93E-08	1.21E-08
	SO_2	Emissions/Waste	kg/h	39.87	13.84	23.36	23.36	23.36	10.25
	SO_3	Emissions/Waste	kg/h	23.69	20.22	22.27	22.27	22.27	13.45
	Water Waste	Emissions/Waste	kg/h	3423.86	2929.18	3105.87	3105.87	3488.16	2764.65
	O_2	Product	kg/h	87.21	87.21	87.21	87.21	87.21	87.21
	Ash	Product	kg/h	107.93	118.06	107.93	107.93	107.93	118.06
	Electric energy	Product	kWh	44779.27	42542.63	40225.99	40324.92	40532.91	39654.26
	HVACs	Product	kg/h	-	-	632.90	592.90	642.18	342.49
	NaCl	Product	kg/h	-	-	-	-	382.29	-
	Spent ZSM-5	Product	kg/h	-	240	-	-	-	2400

Table 14 Composition of recovered HVACs in product streams for scenarios 3,4,5,6.

Stream	Scenario 3 SCOLPROD (%)	Scenario 4 SBTX2 (%)	SPHENOL (%)	SCOOLOXY (%)	SHEAVY (%)	Scenario 5 SLIQCOLD (%)	SPHENCO (%)	Scenario 6 SCOLPROD (%)
AR	0.10	0.35	0.05	0.00	0.00	0.36	0.00	37.23
ALI	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6.08
PH	5.72	9.92	8.79	4.99	0.86	0.00	7.12	14.42
FUR	0.62	1.32	0.99	0.36	0.04	2.21	0.00	0.00
ETH	0.00	0.00	0.00	0.00	0.00	29.64	0.00	0.00
ALD	0.29	0.02	0.03	0.28	0.70	1.04	0.00	0.00
KET	3.46	11.39	2.59	0.22	0.01	12.36	0.00	0.00
PAHs	0.00	0.00	0.00	0.00	0.00	0.00	0.00	16.12
OxyAR	0.77	1.02	1.18	0.90	0.16	2.75	0.00	0.00
OxyPH	74.58	75.96	86.35	93.22	45.71	0.00	92.88	5.18
Un+Sul	14.46	0.02	0.02	0.03	52.52	51.65	0.00	20.97

AR-Aromatics; ALI-Aliphatics; PH-Phenolics; FUR-Furans; ETH-Ethers; ALD-Aldehydes; KET-Ketones; PAHs: Polycyclic aromatic hydrocarbons; OxyAR-Oxygenated Aromatics; OxyPH-Oxygenated Phenoloics; UN+SUL-Unidentified and Sulfur compounds

Table 15 shows the equipment cost per category for the 6 scenarios and Table 16 presents the calculations of the the overall CAPEX and OPEX of the 6 scenarios in MM€.

Table 15. Equipment cost per category for 6 scenarios of lignin pyrolysis oil valorization.

Category	Scenario 1 (€)	Scenario 2 (€)	Scenario 3 (€)	Scenario 4 (€)	Scenario 5 (€)	Scenario 6 (€)
Boiler	1,493,909	1,494,370	1,468,589	1,455,478	1,455,478	1,467,232
Heat Exchanger	12,518,226	11,871,736	11,716,485	11,301,089	11,402,528	11,119,206
Separator	203,124	203,125	40,203,124	388,044	434,100	40,203,125
Pump	73,600	73,600	73,600	73,600	73,600	73,600
Pyrolysis Reactor	152,000	152,000	152,000	152,000	152,000	152,000
Turbine	9,701,426	9,240,858	8,763,817	8,784,188	8,827,017	8,646,086
Tank	25,687	25,687	25,687	25,687	275,233	25,687
Purchase cost (PC)	24,167,972	23,061,376	62,403,302	22,180,086	22,619,956	61,686,936

Table 16. Calculation of the overall CAPEX and OPEX of the 6 scenarios in (MM€).

	Scenario 1	Scenario 2	Scenario 3	Scenario 4	Scenario 5	Scenario 6
Direct Capital Costs (DC)	93.05	88.79	240.25	85.39	87.09	237.49
Total Indirect Capital Costs (IC)	17.88	17.07	46.18	16.41	16.74	45.65
Total Other Capital Costs (OC)	16.92	16.14	43.68	15.53	15.83	43.18
Total Capital Investment (TCI)	**147.03**	**140.29**	**379.63**	**134.93**	**137.61**	**375.27**
A. Manufacturing Cost (MC)	57.30	64.73	101.32	55.06	58.57	109.52
B. General Expenses (GE)	10.45	11.50	19.16	10.10	10.69	20.36
Total Production Cost (TPC)	**67.75**	**76.23**	**120.48**	**65.16**	**69.27**	**129.88**

Table 17 shows the annual revenue per scenario and per product.

Table 17. Annual revenue per product/by-product for 6 scenarios.

	Scenario 1 (MMEUR/yr)	Scenario 2 (MMEUR/yr)	Scenario 3 (MMEUR/yr)	Scenario 4 (MMEUR/yr)	Scenario 5 (MMEUR/yr)	Scenario 6 (MMEUR/yr)
O_2	3.90	3.90	3.90	3.90	3.90	3.90
ASH	0.08	0.09	0.08	0.08	0.08	0.09
Electric Energy	46.68	44.35	41.93	42.04	42.25	41.34
HVACs			230.32	74.50	79.21	238.34
Spent ZSM-5		0.18				0.18
NaCl					0.28	
Sum	50.66	48.51	276.23	120.52	125.72	283.84

The main revenue for scenarios 3 to 6 will come from HVACs with a rate of 30.93 thousand EUR/h, 10.01 thousand EUR/h, 10.64 thousand EUR/h and 32.01 thousand EUR/h respectively with the sold electricity covering the 92.15%, 91.42%, 15.18%, 34.88%, 33.61%, 14.56% of each scenario's respective revenue (scenarios 1-6). The rest of the revenue streams represent a very small part in the revenue mix. Annual revenue per product/by-product for the 6 scenarios is shown in Table 17 while the production costs for all products are shown in Table 18.

Table 18. Production cost of each product/by-product for 6 scenarios.

	unit	Scenario 1 (EUR/unit)	Scenario 2 (EUR/unit)	Scenario 3 (EUR/unit)	Scenario 4 (EUR/unit)	Scenario 5 (EUR/unit)	Scenario 6 (EUR/unit)
O_2	kg	8.02	9.43	2.62	3.24	3.31	2.75
ASH	kg	0.13	0.16	0.04	0.05	0.06	0.05
Electric Energy	kWh	0.19	0.22	0.06	0.08	0.08	0.06
HVACs	kg			21.32	9.12	9.13	42.76
Spent ZSM-5	kg		0.16				0.05
NaCl	kg					0.06	

Figure 19 shows the production cost and break-even point for the production of 1 kg of HVACs in scenarios 3 to 6
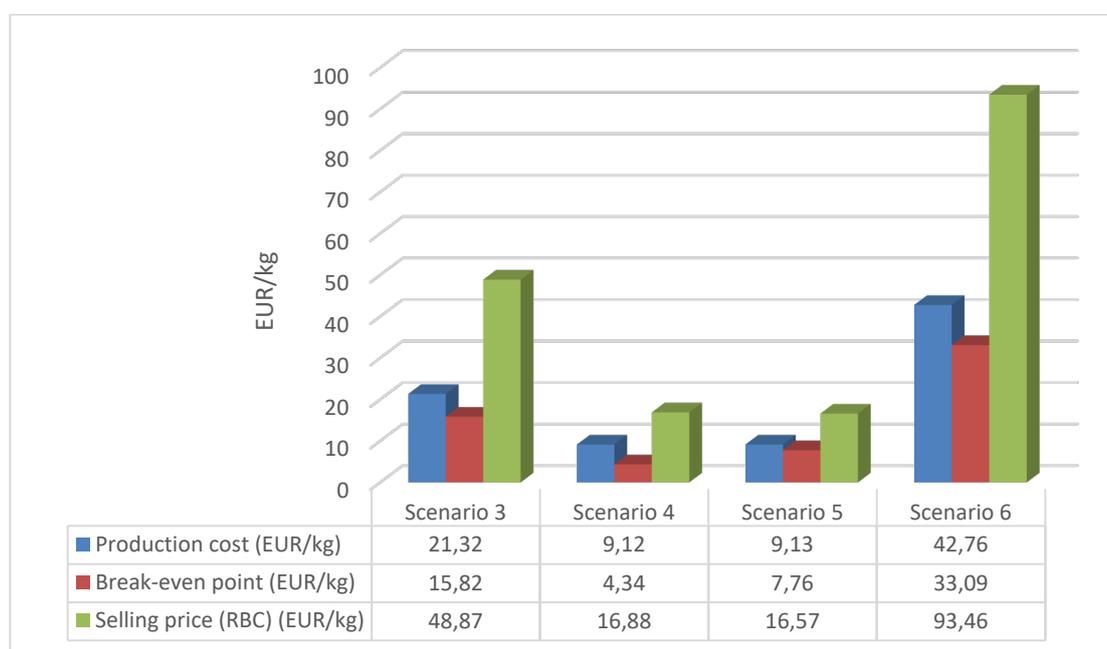
Figure 19. Production cost and break-even point for the production of 1 kg of HVACs in scenarios 3 to 6.

The break-even point for the HVACs is below their production cost due to the multi-product character of the designed plants. To achieve 32% ROI, the respective selling prices for the HVACs in scenarios 3 to 6 are 48.87 EUR/kg, 16.88 EUR/kg, 16.57 EUR/kg and 93.46 EUR/kg (Figure 20).

Conclusions

Based on experimental data, this study offers a techno-economic analysis (TEA) of six (6) scenarios including kraft lignin catalytic (CFP) and thermal (TFP) rapid pyrolysis towards the generation of high value-added chemicals (HVACs) and electric energy. The suggested plants/scenarios were simulated using ASPEN PLUS and custom-based economic models were created in Microsoft Excel. The findings demonstrated that the most cost-effective scenarios are

1 and 2 (no separation section), where the generated bio-oil is utilised as a fuel to generate energy resulting to no profitability. Scenarios 3 and 6 that use the light bio-oil fraction to recover different HVACs and heavier fractions for electricity production have demonstrated a major investment viability. Furthermore, because of the lower separation costs, scenarios 4 and 5, which deal with the recovery of HVAC mixes (fractions), are seen as an intermediate investment alternative. The total capital investment (TCI) for each of the suggested scenarios is significant and ranges from 135 MM€ (scenario 4) to 380 MM€ (scenario 6). According to the comparison of lignin CFP and TFP, the former can produce significant value-added compounds with a lower OPEX than CFP, while the latter can produce aromatic and phenolic monomers with a significant market value. For the HVACs' selling pricing, a 32% return on investment (ROI) target has been established.

4.7. Case 6: Process modelling of chitosan production from dead bees (related to LSIWC→ECORESOURCES secondment)

General

A process modelling of the production of chitosan from dead bees has been performed based on the experimental data shown in Figure 20. The study is ongoing and the results are not finalised.
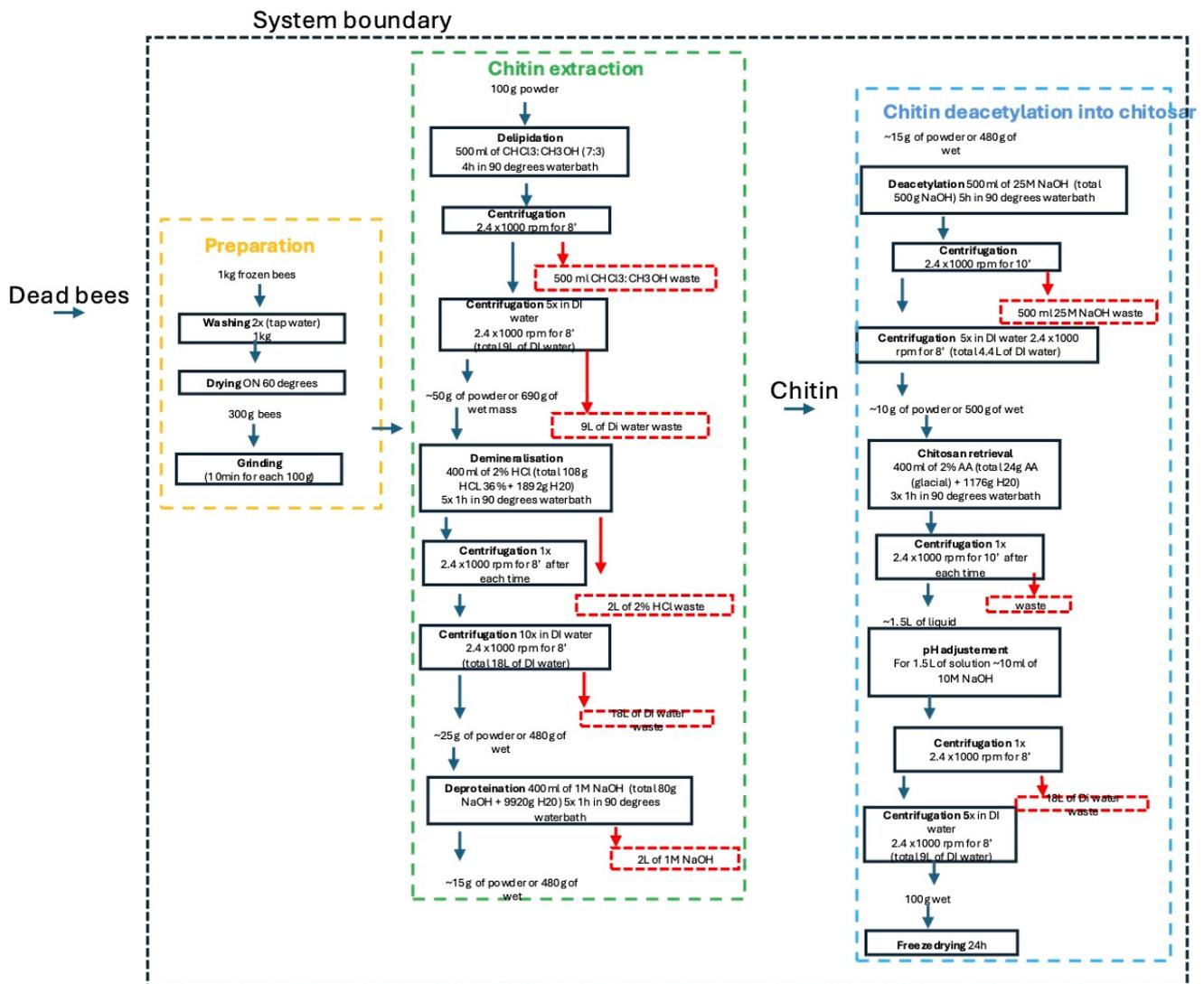
Figure 20. Experimental data for the production of chitosan from dead bees.

The process flowchart is shown in Figure 21.
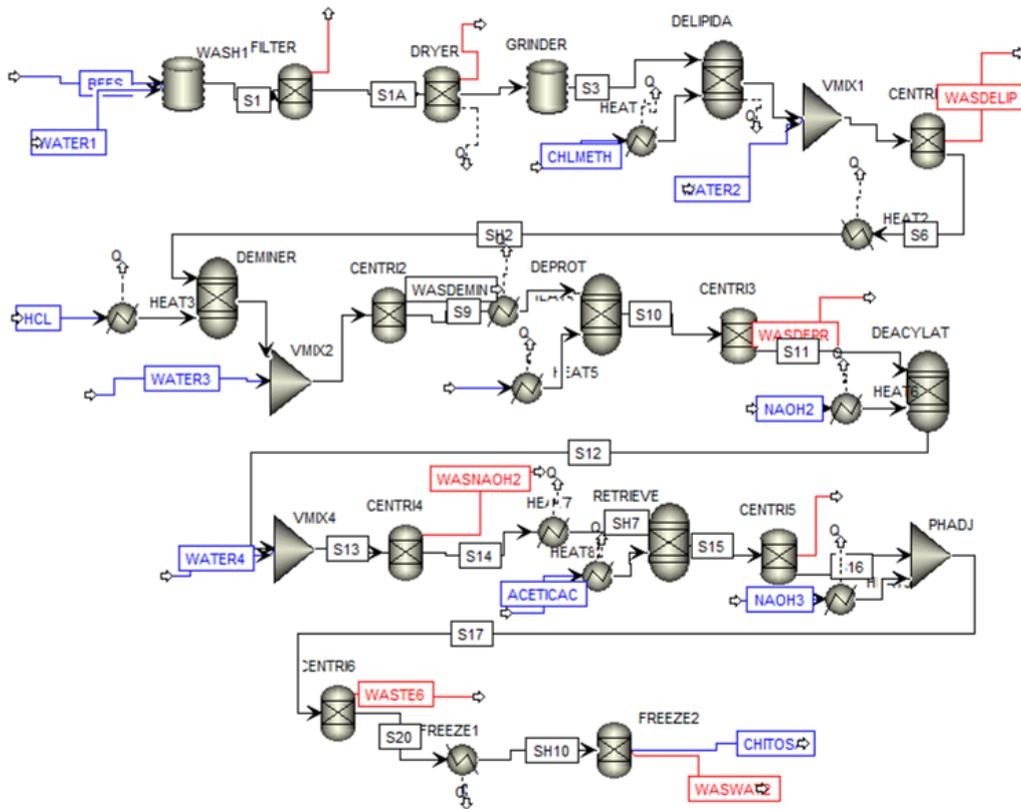
Figure 21. Process flowchart for chitosan production from dead bees.

The results for the material and energy streams are shown in Table 19(In) and Table 20 (out)

Table 19. Materials and energy for chitosan production - In

In	Annual Flow
NAOH (kg/y)	21400.26
HCl (kg/y)	3725.56
CHCl$_3$ (kg/y)	5872.11
METHANOL (kg/y)	6291.72
WATER (kg/y)	2606784.47
ACETIC (kg/y)	13714.29
BEES (kg/y)	16800.00
ENERGY (kwh)	1257428.74

Table 20. Chitosan production - Out

Out	Annual Flow
CHITOSAN (kg/y)	252.47
NAOH (kg/y)	10700.13
HCL (kg/y)	319.33
$CHCL_3$ (kg/y)	5872.11
METHANOL (kg/y)	6291.72
WATER (kg/y)	1502094.89
ACETIC (kg/y)	13440.00
BEES (kg/y)	11256.00
WDELIP (kg/y)	2772.00
WDEPROT (kg/y)	837.14
WRETR (kg/y)	296.38

The initial results regarding the economics of the production of chitosan from dead bees show a CAPEX of 233,192 EUR and OPEX of 251,551 EUR for the production of 252 kg of Chitosan.

Discussion on initial results

Initial results show that the proposed method of chitosan production seems very costly and a lot of optimization on the process and modelling has to be done before reaching actual conclusions.

5. PART C – LIFE CYCLE ASSESSMENT (TASK 2.4)

5.1. Introduction to life cycle assessment (LCA)

Life Cycle Assessment (LCA) is a scientific method used to assess the environmental influences related to a product, process, or carrier for the duration of its complete lifestyles cycle. By quantifying energy use, emissions, resource consumption, and waste generation, LCA offers a systematic approach that helps sustainable decision-making in industry, policy, and research.

The internationally recognized framework for LCA is established by the ISO 14040 series of standards. Specifically, ISO 14040:2006 defines the principles and framework for conducting an LCA, while ISO 14044:2006 provides detailed requirements and guidelines for implementation.

According to these standards, an LCA consists of four main phases:

1.   Goal and Scope Definition – identifying the purpose, system boundaries, and level of detail required.

2.   Life Cycle Inventory (LCI) Analysis – compiling data on inputs (materials, energy, water) and outputs (emissions, waste, products) for each stage.

3.   Life Cycle Impact Assessment (LCIA) – evaluating potential environmental impacts such as climate change, resource depletion, acidification, or human toxicity.

4.   Interpretation – analyzing results to provide clear, consistent conclusions and recommendations for improvement.

A wide range of available software like SimaPro, OpenLCA and others can facilitate (and standardize) the LCIA stage of the LCA.

The report gives a review of the LCAs that have been done using input from WP1 under CELISE project during the various secondments and/or internal research of the parties. Additionally, a systematic approach to transferring knowledge regarding LCA to non-developed rural areas has been proposed. **Specifically, 5 cases are presented:**

Case 1: LCA of bioethanol production from brewer's spent grain

Case 2: Feasibility study (with environmental data) for egg packaging from ecological and biodegradable materials from natural fibres with functional biopolymer additives

Case 3: LCA of HVACs production from lignin pyrolysis

Case 4: LCA of chitosan production from dead bees (bases on initial results)

Case 5: Methodology for transferring knowledge regarding LCA to non-developed rural areas (La Guajira)

5.2. Case 1: LCA of bioethanol production from brewer's spent grain (related to UC→ECORESOURCES secondment)

Introduction

The study is a gate-to-gate life cycle análisis for the production of bioethanol from brewer's spent grain (BSG), a by-product of the beer production process. The results will lead to the assessment

of the main environmental impacts during the biofuel production process, allowing for improvement in the individual processes and their efficiency, and thus minimizing the impact, while promoting the circular economy.

Methodology

The study is conducted in accordance with ISO 14040 and 14044 standards. Calculations were made using OpenLCA (an alternative to SimaPro), with the ReCiPe 2016 midpoint (H) methodology and using the Ecoinvent v3.10 APOS System Processes database for the LCI.

The functional unit of the system is defined as the production of 1 (one) kg of bioethanol from BSG, in order to ensure consistency and allow comparison with other systems.

Figure 22 shows the flowchart of the process on which this study was based while Table 21 shows the input data and Table 22 the output data that were used in the modelling of the process inside OpenLCA
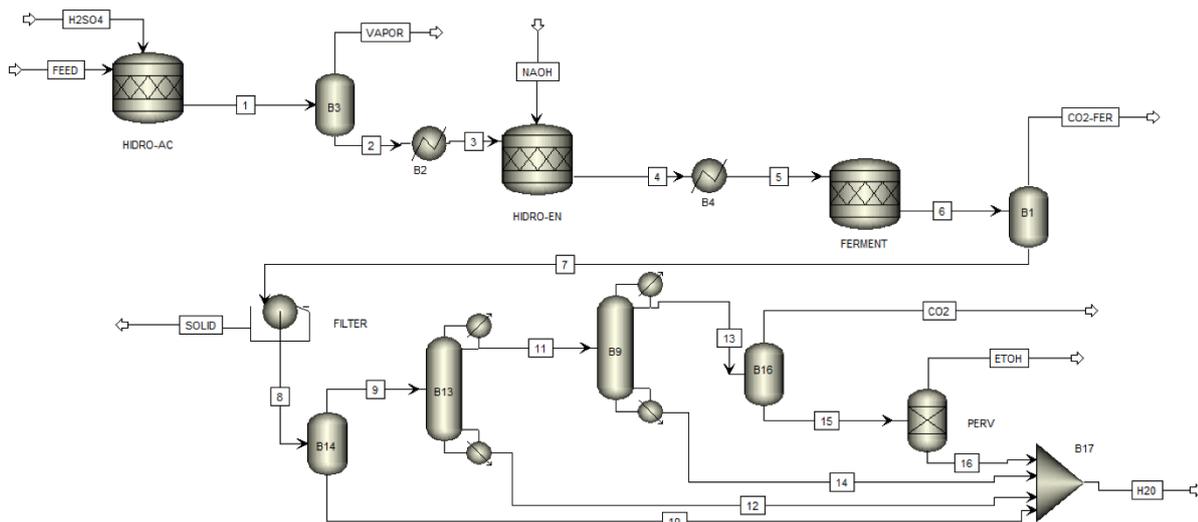
Figure 22. Process Flowchart of biethanol production from BSG.

Table 21. Input data of biethanol production from BSG in OpenLCA

Flow	Category	Amount	Unit
brewer's spent grain	-	24.2	kg
cooling energy	Steam and air conditioning supply	818.49	kWh
electricity, low voltage	Electric power generation, transmission, and distribution	288	kWh
sodium hydroxide, without water, in 50% solution state	Manufacture of basic chemicals	440.37	kg
sulfuric acid	Manufacture of basic precious and other non-ferrous metals	640	kg
tap water	Water collection, treatment, and supply	5173	kg

Table 22. Output data of biethanol production from BSG in OpenLCA

Flow	Category	Amount	Unit
bioethanol	product	3	kg
carbon dioxide, in chemical industry	Manufacture of fertilizers and nitrogen compounds	2.34	kg
steam, in chemical industry	Steam and air conditioning supply	3580	kg
wastewater	-	2692.346	kg

Results and discussion

Table 23 shows the environmental impact of the production of 1kg of bioethanol per impact category. The discusión will focus on the Impact category of climate change for which the environmental impact flow is shown in Figure 23.

Table 23. Environmental impact of 1kg of bioethanol per impact category

Impact category	Result	Reference unit
Acidification: terrestrial	1.263202401	kg SO2-Eq
Climate change	311.4230173	kg CO2-Eq
Ecotoxicity: freshwater	60.22752597	kg 1,4-DCB-Eq
Ecotoxicity: marine	84.13525861	kg 1,4-DCB-Eq
Ecotoxicity: terrestrial	4718.846529	kg 1,4-DCB-Eq
Energy resources: non-renewable, fossil	79.68335583	kg oil-Eq
Eutrophication: freshwater	0.145920969	kg P-Eq
Eutrophication: marine	0.015982508	kg N-Eq
Human toxicity: carcinogenic	76.4098706	kg 1,4-DCB-Eq
Human toxicity: non-carcinogenic	1919.94431	kg 1,4-DCB-Eq
Ionising radiation	29.28409923	kBq Co-60-Eq
Land use	8.088752437	m^2*a *crop-Eq*
Material resources: metals/minerals	6.781959019	kg Cu-Eq
Ozone depletion	0.000253692	kg CFC-11-Eq
Particulate matter formation	0.612223063	kg $PM_{2.5}$-Eq
Photochemical oxidant formation: human health	0.706870345	kg NOx-Eq
Photochemical oxidant formation: terrestrial ecosystems	0.729100742	kg NOx-Eq
Water use	6.588612667	m^3
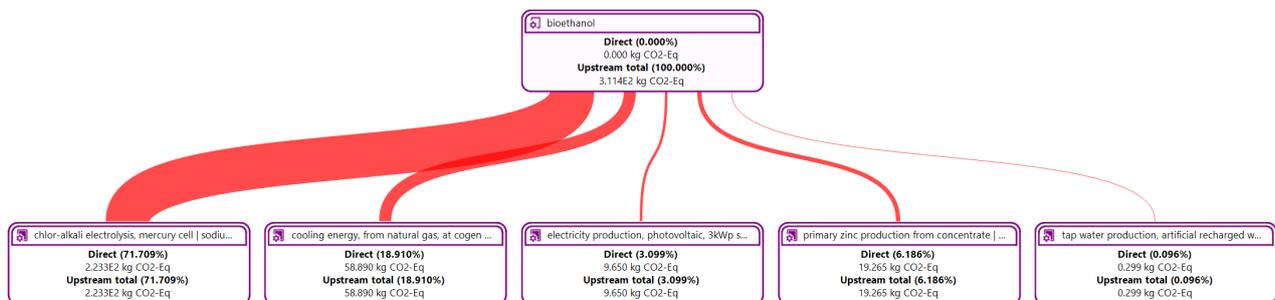
Figure 23. Environmental Impact flow in the Climate Change Category

According to Muñoz et al.[21], CO_2 eq emissions for cradle-to-gate LCA range between 0.7 – 1.5 kg per kg of ethanol produced from sugarcane, sugar beet or corn wheat. The Morales-Vera et al. study[22] on the conversion stage of lignocellulosic biomass (hybrid poplar) gives results on the climate change value equal to 0.24 kg CO_2 eq, while for cradle-to-gate it is equal to approximately 0.27 kg CO_2 eq. In the results of the Shakelly et al.[23] study, which is cradle-to-gate LCA, climate change has a value of 88.95 kg CO_2 Eq for maize, 0.85 kg CO_2 eq for wheat straw, 0.23 kg CO_2 eq for forest residues. The González-García et al.[24] study (cradle-to-grave)

gives values: climate change -0.40 kg CO_2 eq for eucalyptus, -1.83 kg CO_2 eq for pseudoacacia and -0.62 kg CO_2 eq for poplar. In this particular study the emissions in CO_2 equivalents are equal to 311.43 kg per kg of ethanol produced indicating, by comparisson, issues that should be addressed at the modelling or data collection (LCI) stage.

As shown in Figure 25, the production process of caustic sodium, which is used for neutralization in the HIDRO-EN reactor, is the one that mainly contributes to climate change with a percentage of 71.71%. The energy used to cool the system (18.91%) also leads to greenhouse gas emissions, as it comes from natural gas, which is a fossil fuel. The rest of the processes contribute to the greenhouse effect by a much smaller percentage.

To reduce the impact, it is suggested to change the type of energy used, as the production of chemical reagents, such as NaOH, is a process that requires large amounts of energy. Renewable energy instead of fossil fuel-based energy will improve the impacto on the climate change category. Furthermore, the search for alternative chemicals and the optimization of the process so that a smaller quantity of them are required, will lead to reduced effects on environmental impact, though the reassessment of the LCI and of the model is the first thing to address.

Conclusions

This study is an LCA of bioethanol produced from BSG and was based on a process designed at Aspen Plus rather than actual industrial data. The aim is to identify the main environmental impacts based on the impact categories, in order to propose appropriate actions to optimize the production process, reducing the burden on the environment and human health.

Indicatively, some of the resulting results are, for the category: climate change 311.42 kg CO_2 eq, acidification, 1.26 kg SO_2 Eq, soil ecotoxicity 4718.85 kg 1.4-DCB eq, human toxicity (non-carcinogenic) 1919.94 kg 1.4-DCB eq, ozone depletion 0.00025 kg CFC-11 eq, water use 6.59 m^3.

The results show high values for the impact categories, i.e. the bioethanol production process based on the developed flowchart and the inputs of the system, leads to large amounts of emissions and therefore to a great strain on the environment. The main cause of the effects is the synthesis of sodium hydroxide (NaOH), which in the modeling of the data by ecoinvent, is carried out by salt electrolysis and requires high amounts of energy. Therefore, it causes high energy consumption, pollutant emissions and requires management of by-products. The impact categories are therefore affected by climate change, photochemical oxidant formation, ozone depletion, water use. This is followed by the synthesis of sulfuric acid (H_2SO_4) where, based on the input from ecoinvent, it is done by processing zinc ores. This process leads to CO_2, SO_2 and heavy metal emissions, as it also requires high amounts of energy. As a result, there are increased impacts on climate change, acidification, photochemical oxidant formation, ecotoxicity. The cooling process of the system is modeled using energy derived from natural gas and affects

the impact category of energy and material resources. It is worth noting that the other processes also contribute to the impact, but at a smaller percentage.

To reduce the environmental footprint of bioethanol production, it is necessary to:

- Review the flow chart design at Aspen Plus, and the processes it includes to improve the efficiency of fermentation and distillation to reduce water and energy consumption
- Use renewable energy sources such as solar or wind instead of fossil fuel-based energy to reduce greenhouse gas emissions and prevent the depletion of energy resources as much as possible
- To test alternative chemical reagents, analogous to NaOH and H_2SO_4, reducing the depletion of mineral resources, and apply different stages of pre-treatment, which will lead to lower environmental impacts
- Implement a circular economy, in which the waste of one process is recycled and appropriately used as inputs to other processes.

5.3. Case 2: Feasibility study (with environmental data) for egg packaging from ecological and biodegradable materials from natural fibres with functional biopolymer additives

The aim of feasibility study was to assess and evaluate, which type fibre product is most promising from technical and economic aspects to develop up to TRL 6 within the project "Development of ecological and biodegradable materials from natural fibres with functional biopolymer additives "EcBioMa", which is being implemented via effective cooperation of scientific institution Latvian State Institute of Wood Chemistry and moulded fibre producing company SIA V.L.T. It was necessary to review several important aspects, such as technical, financial, environmental, market demands, market potential, customer buying habits, current and potential competitors and others. In has to be noted that study was very important from a very practical point of view to decide, if pilot line of R&D department of company V.L.T. has to be updated with different moulds in order to develop new and improved products within the project.

Feasibility study report contains description of state of the art of manufacturing process of moulded fibre products (MPP), including classification of products, history, review of applications, conventional and non-conventional raw materials, tooling of products, most important properties. A lot of attention has been paid to the environmental aspects, taking into account environmental impact of MPP production and end-life. Existing requirements and regulations regarding production, waste management, climate change, emissions, circular economy, and other aspects have been evaluated. Consumer behaviour, market demand and forecasts, competition in the market have been evaluated as well. Study contains business overview of company V.L.T., showing its economic and technical possibilities and potential. SWOT analysis and risk assessment of MPP packaging have been carried out and presented.

It has been concluded that improved egg packaging - MPP made from wastepaper fibres with minor addition of virgin fibres of various origin, and bio-polymer additives for improvements of

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mechanical properties in dry and wet state should be developed within the project up to TRL 6, including preliminary stage at laboratory scale equipment. It was concluded also that it is necessary to update production line used for R&D activities with appropriate moulds with improved functionality, and to carry on preliminary development stages of improved MPP product at laboratory scale in order to prevent failures at industrial scale pilot lines.

More information can be found here.

5.4. Case 3: LCA of HVACs production from lignin pyrolysis

Introduction

Cradle to gate LCA studies were conducted for the 6 scenarios of utilization of Kraft lignin through catalytic pyrolysis for electricity generation and HVACs recovery as described in the chapter 4.6.

The functional unit (FU) used for energy production is 1kWh and 1kg for the recovered chemicals. For the analysis of the entire process in each scenario, the production of energy and HVACs in one hour (1 h) of operation of the unit (functional unit) was studied.

Methodology

The calculations were based on mass and energy balances calculated during the techno-economic analysis stage (chapter 4.6).

The LCAs were carried out in the context of product qualitative comparison using SimaPro v7.3.3, the ReCiPe Midpoint (H) V1.06/ Europe method and the EcoInvent v.3 and ELCD databases.

Kraft lignin was produced with Lignoboost technology and was entered into the SimaPro database with data found in the literature[25,26].

For the products that are recycled during the process of each scenario and given that all quantities are renewed annually (see techno-economic study assumptions), in addition to the quantity of the new material, a quantity corresponding to the production of 1 unit (h, kg or kWh) were calculated. Thus, the sand that is recycled at a rate of 100% in scenario 1 participates in the LCA with 0.805801773 kg per hour (6000kg/7446h).

It is assumed that electricity is the source of energy for the production processes of Kraft Lignin. This would be done on an industrial scale by using natural gas or steam which would potentially have a lower cost and lower absolute environmental impact.

Given that the process of (catalytic) lignin pyrolysis for the recovery of HVACs in combination with electricity generation is a relatively new subject and due to this there is limited relevant literature for comparison, the results should be used for comparisons within the boundaries of this study in the context of the evaluation of the different scenarios and not as absolute figures for decision-making on environmental issues by public or private entities.

For the implementation of the LCAs, the following processes had to be added manually to the SimaPro database:

- Kraft Lignin (All Scenarios). Production of 1 kg.
- Electric energy (All Scenarios). Production of 1 kWh
- HVACs (Scenarios 3, 4, 5, 6). Production of 1kg
- Ash. From 1kWh of enrgy (Scenarios 1, 2) or 1 kg of HVACs (Scenarios 3, 4, 5, 6)
- Oxygen. From 1kWh of enrgy (Scenarios 1, 2) or 1 kg of HVACs (Scenarios 3, 4, 5, 6)
- NaCl. From the production of 1 kg HVACs (Scenario 5)

In addition, 6 scenarios were added as a collection of assemblies for 1 hour of runtime of the plant of each scenario.

The categories in which each type of compound, material or energy used in the LCAs relate to the input in SimaPro are as follows:

   i.   Outputs to technosphere
   ii. Inputs from nature – resources
   iii. Inputs from technosphere - materials
   iv. Inputs from technosphere - energy
   v.   Emissions to air
   vi. Emissions to water
   vii. Final waste flows
   viii. Waste and emissions to treatment

Table 24 shows the input/output data for the 6 scenarios of Kraft lignin pyrolysis to 1 kWh electric energy and 1 kg HVACs and Table 25 shows the Output data for 1h of runtime.

Table 24. Input/output data for the 6 scenarios of Kraft lignin pyrolysis to electric energy (1 kWh FU) and HVACs (1 kg FU).

in/out	type	Category	Units	Scenario 1	Scenario 2	Scenario 3	Scenario 4	Scenario 5	Scenario 6
Out	CO_2	v	kg	0.331208017	0.345932444	20.98727102	22.40316731	20.6864732	40.39919755
Out	O_2	v	kg	0.003413695	0.004317124	0.13392483	0.142960005	0.132005366	0.783393014
Out	NO_2	v	kg	8.13611E-08	1.02125E-07	3.19485E-06	3.41039E-06	3.14906E-06	1.87925E-05
Out	NO	v	kg	1.91323E-06	2.18847E-06	9.95291E-05	0.000106244	9.81027E-05	0.000338604
Out	CO	v	kg	9.57243E-12	8.53292E-12	6.71136E-10	7.16414E-10	6.61517E-10	6.59389E-10
Out	N_2	v	kg	0.928088407	0.954895218	58.63747886	62.59342859	57.79706349	109.480011
Out	H_2	v	kg	6.85673E-13	5.20987E-13	4.81268E-11	5.13737E-11	4.74371E-11	3.57178E-11
Out	Water from burner	viii	kg	0.076176209	0.069863386	4.907334251	5.238405231	5.432366415	8.072126021
Out	Water for Rankine cycle	vi	kg	0.00068724	0.000685257	0.043924755	0.046888118	0.043295208	0.080385524
Out	Cooling water	vi	kg	9.223878488	9.202268343	592.1646246	629.2888109	579.545119	1082.560299
Out	O_2 (sell)	i	kg	0.001940399	0.00196037	0.137800119	0.147096738	0.135825113	0.254644662
Out	Ash	i	kg	0.002401336	0.002561562	0.170534206	0.182039215	0.168090043	0.344713451
Out	Electric energy (sell)	i	kWh	1	1	63.80433402	68.10886318	63.36803172	117.2782393
Out	Sand or ZSM-5	vii	kg	1.7928E-05	1.81125E-05	0.001273181	0.001359076	0.001254934	7.016832755
Out	HVACs	i	kg	-	-	1	1	1	1
Out	NaCl	i	kg	-	-	-	-	-	-
In	Lignin	iii	kg	0.133491826	0.134865743	9.480107938	10.11967893	9.344235308	17.51855442
in	Sand or ZSM-5	iii	kg	1.7928E-05	1.81125E-05	0.001273181	0.001359076	0.001254934	7.016832755
In	Air	ii	kg	1.209738232	1.244666651	76.43113735	81.58752782	75.33569627	142.6990983
In	Electric energy (buy)	iv	kWh	0.000998143	0.001005817	0.458168538	0.083448198	0.151028985	0.846437411
In	Water for Rankine cycle	iii	kg	0.00068724	0.000685257	0.043924755	0.046888118	0.043295208	0.080385524
In	Cooling water	iii	kg	9.223878488	9.202268343	592.1646246	629.2888109	579.545119	1082.560299
In	AcOEt	iii	kg	-	-	0.031950147	-	-	0.059041563
In	Hexane	iii	kg	-	-	0.031250572	-	-	0.0577488
In	DEE	iii	kg	-	-	-	-	0.076627295	-
In	NaOH	iii	kg	-	-	-	-	0.622904012	-
In	HCl	iii	kg	-	-	-	-	0.567827999	-

D2.2. Mathematical tools in small biorefineries:
artificial neural network models, simulation and
optimization and LCA

Table 25. Output data for 1h of runtime.

Type	Scenario1	Scenario 2	Scenario 3	Scenario 4	Scenario 5	Scenario 6
Energy(sell) (kWh/h)	44946.57	44488.69	40382.03	40382.03	40689.06	40167.09
Ash (kg/h)	107.93	113.96	107.93	107.93	107.93	118.06
Oxygen (kg/h)	87.21	87.21	87.21	87.21	87.21	87.21
HVACs (kg/h)	-	-	632.90	592.90	642.11	342.49
NaCl (kg/h)	-	-	-	-	382.29	-

Table 26 shows the impact allocation for the products of all scenarios.

Table 26. Impact allocation

	Scenario 1	Scenario 2	Scenario 3	Scenario 4	Scenario 5	Scenario 6
O_2	7.66%	7.74%	2.09%	4.36%	4.22%	1.34%
Ash	0.16%	0.17%	0.04%	0.09%	0.09%	0.03%
Electric energy	92.18%	92.09%	22.61%	47.08%	45.98%	14.41%
HVACs			75.26%	48.47%	49.68%	84.22%
Nacl					0.03%	
Total	100%	100 %	100%	100%	100%	100%

Results

Table 27 shows the envirnmental impact per category for the production of 1kWh of electric energy at scenarios 1 and 2.

Table 27. Environmental impact per category for the production of 1kWh of electric energy at scenarios 1 and 2

Impact category	Unit	Scenario 1	Scenario 2
Climate change	kg CO_2 eq	1.94338614	2.134294479
Ozone depletion	kg CFC-11 eq	1.8984E-07	2.08502E-07
Human toxicity	kg 1.4-DB eq	0.82618917	0.934489247
Photochemical oxidant formation	kg NMVOC	0.01491779	0.015837016
Particulate matter formation	kg PM10 eq	0.00612809	0.006601525
Ionising radiation	kg U235 eq	0.55301357	0.614372131
Terrestrial acidification	kg SO_2 eq	0.01423037	0.015234812
Freshwater eutrophication	kg P eq	0.00073473	0.000829192
Marine eutrophication	kg N eq	0.00133674	0.001423561
Terrestrial ecotoxicity	kg 1.4-DB eq	0.00034705	0.000376613
Freshwater ecotoxicity	kg 1.4-DB eq	0.01859709	0.0211367
Marine ecotoxicity	kg 1.4-DB eq	0.01477392	0.017246525
Agricultural land occupation	m^2a	20.9278587	21.75889442
Urban land occupation	m^2a	0.35240045	0.367256049
Natural land transformation	m^2	0.00275152	0.002885311
Water depletion	m^3	0.11342808	0.118641228
Metal depletion	kg Fe eq	0.11586367	0.133451398
Fossil depletion	kg oil eq	0.60419143	0.665400893

Table 28 shows the characterization results of scenarios 3-6 for the production of 1 kg of HVACs in the studied impact categories.

Table 28. Characterization results of scenarios 3-6 for the production of 1 kg of HVACs

Impact category	Unit	Scenario 3	Scenario 4	Scenario 5	Scenario 6
Climate change	kg CO_2 eq	113.4817344	77.6258667	74.50934773	259.1214441
Ozone depletion	kg CFC-11 eq	1.10581E-05	7.58117E-06	7.65293E-06	2.5321E-05
Human toxicity	kg 1.4-DB eq	48.49505641	32.98447909	31.80014072	117.014232
Photochemical oxidant formation	kg NMVOC	0.867174673	0.595181653	0.565840074	1.864154015
Particulate matter formation	kg PM10 eq	0.356412353	0.244493006	0.232820247	0.787599957
Ionising radiation	kg U235 eq	32.11356113	22.06247085	21.13983042	75.14850481
Terrestrial acidification	kg SO_2 eq	0.828394925	0.567923432	0.541777344	1.808788377
Freshwater eutrophication	kg P eq	0.043520955	0.029344558	0.028255645	0.104461374
Marine eutrophication	kg N eq	0.077831999	0.053318254	0.050714383	0.168143106
Terrestrial ecotoxicity	kg 1.4-DB eq	0.020192655	0.013854594	0.013412592	0.045240323
Freshwater ecotoxicity	kg 1.4-DB eq	1.091402055	0.742260278	0.709778593	2.656413252
Marine ecotoxicity	kg 1.4-DB eq	0.869496148	0.589853638	0.567579469	2.216252384
Agricultural land occupation	m2a	1213.510214	834.2632198	789.5830898	2510.001784
Urban land occupation	m2a	20.43603642	14.04867382	13.2986147	42.46003616
Natural land transformation	m2	0.159697492	0.109717957	0.103897842	0.335718662
Water depletion	m3	6.530365796	4.4860274	4.250123789	13.73760896
Metal depletion	kg Fe eq	6.732065241	4.623412945	4.41717512	16.80273072
Fossil depletion	kg oil eq	35.32194882	24.14601869	23.14825927	81.19844687

Table 29 shows the environmental impact of 1h of runtime for the 6 scenarios per impact category.

Table 29. Environmental impact (characterization) of 1h of runtime

| Impact category	Unit	Scenario 1	Scenario 2	Scenario 3	Scenario 4	Scenario 5	Scenario 6
Climate change	kg CO_2 eq	94758.3105	100105.3550	95432.6776	94954.4971	96292.8614	105375.2961
Ozone depletion	kg CFC-11 eq	0.0093	0.0098	0.0093	0.0093	0.0099	0.0103
Human toxicity	kg 1.4-DB eq	40284.4748	43830.5861	40782.0087	40347.6928	41097.2131	47585.4455
Photochemical oxidant formation	kg NMVOC	727.3821	742.8076	729.2522	728.0456	731.2688	758.0838
Particulate matter formation	kg PM10 eq	298.8020	309.6330	299.7256	299.0718	300.8875	320.2883
Ionising radiation	kg U235 eq	26964.6007	28816.0518	27005.9595	26987.5354	27320.2601	30560.1722
Terrestrial acidification	kg SO_2 eq	693.8641	714.5622	696.6403	694.7025	700.1711	735.5687
Freshwater eutrophication	kg P eq	35.8250	38.8918	36.5990	35.8952	36.5165	42.4807
Marine eutrophication	kg N eq	65.1784	66.7697	65.4530	65.2206	65.5412	68.3777
Terrestrial ecotoxicity	kg 1.4-DB eq	16.9217	17.6644	16.9811	16.9474	17.3339	18.3976
Freshwater ecotoxicity	kg 1.4-DB eq	906.7827	991.3800	917.8166	907.9570	917.2891	1080.2670
Marine ecotoxicity	kg 1.4-DB eq	720.3671	808.9181	731.2044	721.5282	733.5167	901.2695
Agricultural land occupation	m^2a	1020429.4923	1020562.9413	1020503.6926	1020498.0358	1020425.1860	1020726.7181
Urban land occupation	m^2a	17182.8290	17225.5036	17185.7232	17184.7970	17186.5907	17266.9572
Natural land transformation	m^2	134.1623	135.3305	134.2979	134.2106	134.2734	136.5246
Water depletion	m^3	5530.6831	488.0932	5491.7234	5487.4553	5492.6877	5586.5875
Metal depletion	kg Fe eq	5649.4414	126.2005	5661.3429	5655.5098	5708.5781	6833.0614
Fossil depletion	kg oil eq	29460.0016	3849.8144	29704.0592	29536.1992	29915.8722	33020.4643
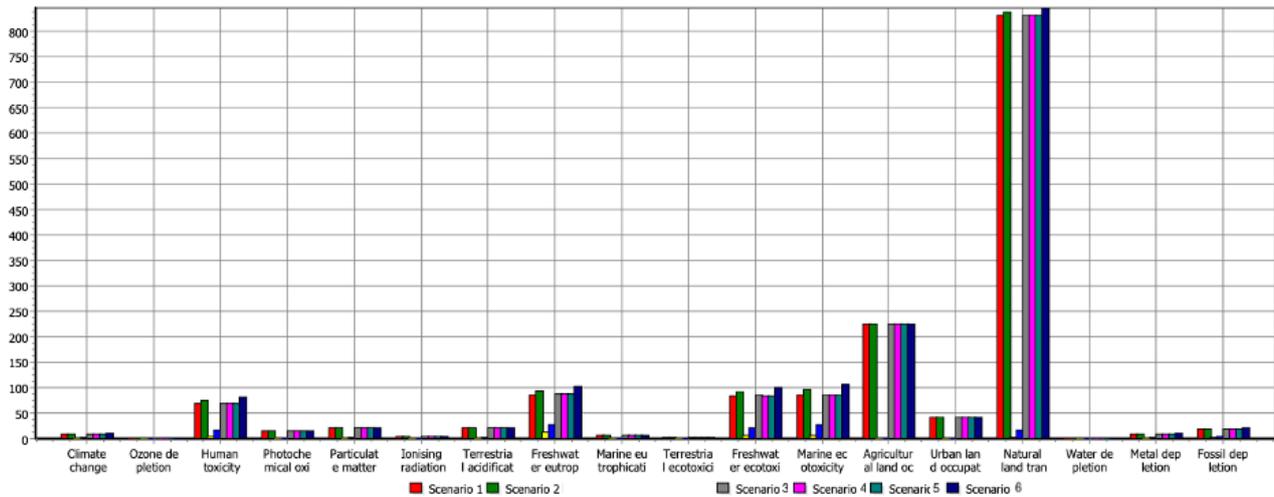
Figure 24. Normalization results of the environmental imapct for 1h of runtime

The results (Table 27) show that the production of 1 kWh of energy from the catalytic pyrolysis of kraft lignin has the more intense environmental impact of the 2 cases in all impact categories. The impact on climate change, which is the main category of impacts examined is 1.94 kg CO_2eq and 2.13 kg kg CO_2eq respectively in the 2 scenarios as shown in the table.

As shown in Table 28, the use of simulated moving bed (SMB) chromatography for the HVACs separation in combination with catalytic pyrolysis is the scenario that brings the greatest environmental impact throughout scenarios 3 to 6. This is followed by the use of SMB after thermal pyrolysis of lignin. Distillation and liquid-liquid extraction seem to have similar environmental impact in most categories. It should be emphasized that, unlike in the case of SMB, extraction and distillation do not achieve the separation of bio-oil into distinct high-purity compounds but bio-oil fractions containing groups of chemical compounds. The LCA demonstrates the high impact of all scenarios on natural land transformation and on agricultural land occupation, which are the impact categories with the highest values in all scenarios. This is due to the raw material (kraft lignin) used which is produced from the processing of tree wood. The impacts on climate change are 113.48 kg CO2eq, 77.63 kg CO2eq, 74.51 kg CO2eq and 259.12 kg CO2eq respectively for scenarios 3 to 6

From the results of the comparison of the operation of one hour in each scenario it appears that, when normlized, the main environmental impacts of the units are, primarily, natural land transformation followed by the use of agricultural land occupation. This is mainly due to the raw material (lignin). The catalytic processes have a higher overall environmental impact, but not with a large difference as it appears in the relevant differences do not have a deviation of more than 10%. Exceptions are human toxicity, freshwater ecotoxicity, marine ecotoxicity and fossil depletion, where again the differences are in the 15% range. The specific impacts, in addition to metal depletion, are also the basic impacts in absolute terms for all processes.

5.5. Case 4: LCA of chitosan production from dead bees (based on initial results-related to LSIWC→ECORESOURCES secondment)

Introduction

An initial calculation of the environmental impact of the production of 1kg of Chitosan from dead bees using data from the initial model (see Chapter 4.8) has been performed. The study is not complete and only the initial results are reported.

Methodology

The calculations were performed using the OpenLCA software, the Ecoinvent 3 database and ReCiPe 2016 Midpoint (H) (v1.03) as the method of calculating the environmental impact.

Table 30 shows the Input-output data used for the calculations.

Table 30. Input-output data – Chitosan production

Input	Amount	Unit
acetic acid, without water, in 98% solution state	54.3204567	kg
Bees	66.5425595	kg
chloroform	23.2586446	kg
electricity, medium voltage	9.6823385	kWh
hydrochloric acid, without water, in 30% solution state	14.756463	kg
methanol	24.9206638	kg
sodium hydroxide, without water, in 50% solution state	84.7635945	kg
water, deionised	10325.1256	kg
	0	
	0	
Output	**Amount**	**Unit**
Ulla's Chitosan	1	kg
sewage sludge, 97% water, WWT-SLF, municipal solid waste	6154.7103	kg

Results

The the results of the initial calculation are presented in Table 31.

Table 31. Environmental impact results by category – Chitosan from bees

Impact category	Unit	Value
Acidification: terrestrial	kg SO2-Eq	778.2331
Climate change	kg CO2-Eq	169011.7
Ecotoxicity: freshwater	kg 1,4-DCB-Eq	5366.859
Ecotoxicity: marine	kg 1,4-DCB-Eq	8052.731
Ecotoxicity: terrestrial	kg 1,4-DCB-Eq	1141245
Energy resources: non-renewable, fossil	kg oil-Eq	33637.43
Eutrophication: freshwater	kg P-Eq	67.17087
Eutrophication: marine	kg N-Eq	190.4613
Human toxicity: carcinogenic	kg 1,4-DCB-Eq	29438.25
Human toxicity: non-carcinogenic	kg 1,4-DCB-Eq	1265562
Ionising radiation	kBq Co-60-Eq	5716.744
Land use	m2*a crop-Eq	2887.889
Material resources: metals/minerals	kg Cu-Eq	902.9796
Ozone depletion	kg CFC-11-Eq	6.133661
Particulate matter formation	kg PM2.5-Eq	299.9372
Photochemical oxidant formation: human health	kg NOx-Eq	361.9478
Photochemical oxidant formation: terrestrial ecosystems	kg NOx-Eq	375.7115
Water use	m3	1778.061

Conclusions

As is the TEA of the process, the LCA study is at its infancy and is by no means a finalized study and no actual conclusions can be reached.

5.6. Case 5: Methodology for transferring knowledge regarding LCA to non-developed rural areas (La Guajira) (related to AUTH→BESARTE secondment)

Introduction

A methodology for transferring knowledge regarding LCA to non-developed rural areas has been presented in the IV International Congress on Biorefineries and Renewable Energies - BERSTIC 2024, with the title "Teaching Life Cycle Assessment (LCA) as a simple process in everyday life". The study focused on teaching the value of LCA to indigenous people of La Guajira, Colombia (Wayuu).

Methodology

Transferring technical tools such as Life Cycle Assessment (LCA) into non-developed or rural regions requires considerations not only to infrastructure limitations but also to cultural, social, and economic realities. La Guajira, a semi-arid region in northern Colombia with strong Indigenous Wayuu presence, offers both opportunities and challenges for LCA adoption.

1. **Local Context and Cultural Considerations**.
   Community Structure: Many communities in La Guajira operate through traditional authorities such as Wayuu clans and elders. Knowledge transfer should respect these structures, engaging leaders and ensuring collective decision-making.
   Language and Communication: While Spanish is spoken, many Wayuu communities use Wayuunaiki. Translating core LCA concepts into local language and using metaphors tied to daily life (e.g., water cycles, weaving, agriculture) can enhance understanding.
   Oral Traditions: Training should rely less on long written materials and more on storytelling, visual diagrams, and participatory workshops. Demonstrations and analogies grounded in lived experience resonate more effectively.
   Trust and Reciprocity: External experts should avoid a "top-down" approach. Co-creation of knowledge, acknowledging local ecological wisdom (e.g., sustainable grazing, water harvesting practices), makes LCA more relevant and respectful.

2. **Practical Barriers and Adaptations**
   Low Infrastructure: Limited internet and electricity mean training methods should be portable (e.g., printed infographics, solar-powered tablets, offline data tools).
   Educational Diversity: Literacy and numeracy levels vary. Using intuitive symbols (red/green arrows for impacts, circles for resource cycles) helps bridge knowledge gaps.
   Relevance to Daily Life: Abstract global impact categories (e.g., global warming potential) should be linked to visible local concerns such as water scarcity, land degradation, or health impacts from mining.

3. **Strategies for Effective Knowledge Transfer.**
   Engagement Through Local Leaders: Train community members who can act as facilitators, ensuring long-term continuity and adaptation of LCA tools.
   Participatory Data Gathering: Engage locals in collecting life cycle data (e.g., fuel use, crop yields, waste handling) to build ownership and contextual accuracy.
   Blending Scientific and Indigenous Knowledge: Integrating traditional ecological practices into LCA frameworks increases legitimacy and enriches the analysis.
   Cultural Anchoring: Relating LCA to cultural symbols (e.g., weaving as a metaphor for interconnected cycles) makes the methodology more accessible.

Sample slides from the presentation are shown in Figures 25-27.

Figure 25. Presentation "Teaching Life Cycle Assessment (LCA) as a simple process in everyday life" – cover.
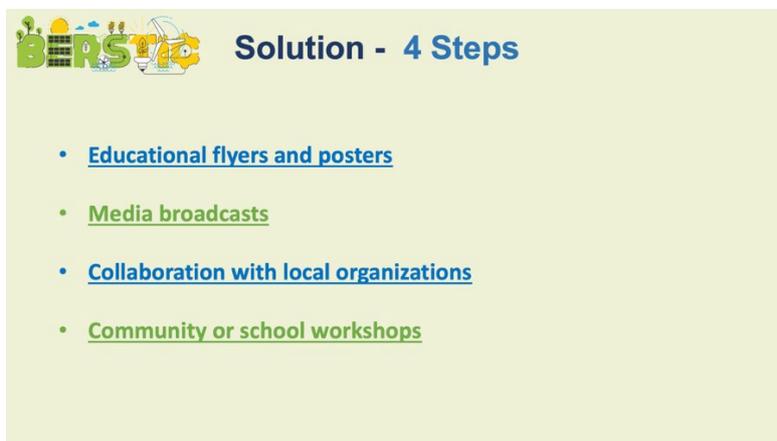

Figure 26. Presentation "Teaching Life Cycle Assessment (LCA) as a simple process in everyday life" – Methodology.

Figure 27. Presentation "Teaching Life Cycle Assessment (LCA) as a simple process in everyday life" – 4 steps.

Conclusions

Effective transfer of LCA knowledge in regions like La Guajira requires more than technical training—it needs cultural respect, participatory methods, and practical adaptation. By combining scientific frameworks with local customs, languages, and priorities, LCA can become a tool for advancement rather than an external imposition.

6. CONCLUSIONS

This report presents the results of various studies performed for the three tasks (Tasks 2.2, 2.3, 2.4) under WP2 of CELISE project in the areas of Artificial neural network models, simulation and optimisation and LCA. The studies were performed during the various secondments under CELISE and/or from internal work of the partners.

Two (2) studies were presented in Artificial Neural Networks (ANNs), 6 studies on Simulation and optimisation (including techno-economic analyses and feasibility studies) and 5 studies on LCA (including feasibility studies containing environmental data) including a methodology of transfering LCA knowledge to rural areas.

Brewers' Spent Grain (BSG) and Ulva rigida represent abundant, low-cost residues with strong potential for circular bioeconomy applications. Experimental and modelling studies confirm that both feedstocks can be converted into fermentable sugars suitable for bioethanol and biobutanol production, though hydrolysis remains the most energy- and cost-intensive stage. Simulation results indicate modest but scalable yields, requiring integration across multiple facilities and co-production of high-value compounds (e.g., ulvan) to improve economic feasibility. Together, these works demonstrate that valorisation of agro-industrial and marine residues can contribute to sustainable fuel alternatives and diversify Europe's renewable energy portfolio. Similar conclusions can be derived from the feasibility study regarding lignocellulosic loose-fill thermal insulation material. The the techno-economic of biomass fractionation and treatment shows that hydrothermal pretreatment of lignocellulosic biomass is the most economical option, with CAPEX about 16% lower than organosolv and significantly lower production costs for lignin biooil. The techno-economic analysis of Kraft lignin fast (catalytic) pyrolysis for the production of high value-added chemicals (HVACs) show that there is a potential for economic viability in the valorization of Kraft lignin pyrolysis, however, the need for advancing the TRL of the process, is the most important parameter that needs to be addressed. The initial process modelling of chitosan production from dead bees shows that there is work needed to reach conclusive results regarding the feasibility of a potential investment on the process.

The LCA study on bioethanol production from BSG show that a revision of the the flow chart design at Aspen Plus is needed, as well as the the processes it includes to improve the efficiency of fermentation and distillation in order to reduce water and energy consumption which appear to be the main factors impacting the environment. The feasibility study for for egg packaging from ecological and biodegradable materials from natural fibres with functional biopolymer additives concludes that it is necessary to update the production line used for R&D activities with appropriate moulds with improved functionality, and to carry on preliminary development stages of improved MPP product at laboratory scale in order to prevent failures at industrial scale pilot lines. The LCA of HVACs production from lignin pyrolysis shows that the main environmental impacts of the units are, primarily, natural land transformation followed by the use of agricultural land occupation due to the raw material (lignin). Also, though the catalytic processes have a slightly higher overall environmental impact with a deviation of no more than 10%. The results of the LCA for the production of phenolic and furanic fractions/compounds from biomass show that the hydrothermal pretreatment of biomass has a lower environmental impact than the organosolv pretreatment for their production, in all categories examined. No actual conclusions can be derived by the LCA of chitosan production from dead bees which is base on initial results of the process modelling. Finally, it has been presented that effective transfer of LCA knowledge in rural areas, is posible and requires more than technical training as it also needs cultural respect, participatory methods, and practical adaptation.

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