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GREEN-LOOP

Sustainable manufacture systems towards novel bio-based materials

WP2 – Sustainability and Circularity by design

D2.2 – Energy, exergy, LCA, SLCA and LCC assessments

Version 1.0

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Consortium	17 organizations: 15 from EU Member States + 2 from UK

GREEN LOOP Consortium Partners

	Partner	Acronym	Country
1	IDENER RESEARCH & DEVELOPMENT	IDE	ES
2	NATIONAL INSTITUTE OF CHEMISTRY	NIC	SI
3	SLOVENIAN NATIONAL BUILDING AND CIVIL E. I.	ZAG	SI
4	FRAUNHOFER GESELLSCHAFT ZUR FOERDERUNG DER ANGEWANDTEN FORSCHUNG E.V	FHF	DE
5	LABRENTA SRL	LBRT	IT
6	MIXCYCLING SRL	MYX	IT
7	NERO SU BIANCO	NSB	IT
8	GERACE MARIA CRISTINA - TERRE DI ZOE’	TDZ	IT
9	IRIS TECHNOLOGY SOLUTIONS, SOCIEDAD LIMITADA	IRIS	ES
10	GLOWNY INSTYTUT GORNICTWA	GIG	PL
11	AACHEN UNIVERISTY: PROCESS CONTROL ENGINEERING / AACHEN UNIVERISTY: INSTITUTE OF SOCIOLOGY	AAU	DE
12	AUSTRIAN STANDARDS INTERNATIONAL	ASI	AT
13	INSTITUTO DE SOLDADURA E QUALIDADE	ISQ	PT
14	AXIA INNOVATION UG	AXIA	DE
15	ASOCIACIÓN DE INVESTIGACIÓN METALÚRGICA DEL NOROESTE	AIMEN	ES
16	NATIONAL COMPOSITE CENTER	NCC	UK
17	UNIVERSITY OF BRISTOL	UBRIS	UK

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Executive Summary

The present document, deliverable **D2.2 – ‘Energy, exergy, LCA, SLCA and LCC assessments’** is focused on GREEN-LOOP’s tasks **T2.2 – ‘Energy and Exergy analysis of the systems’** and **T2.3 – ‘Tools and methodology for LCA, LCC, and Social LCA assessments’** developed within the activities of WP2. The main objectives of these tasks are to analyse the energy transformation in terms of quantity and quality, and to assess the environmental impact and costs of the different products manufactured at both laboratory and industrial scales. This initial deliverable will exclusively present findings from the laboratory scale, with comprehensive industrial scale analysis scheduled for inclusion in Deliverable D2.3, to be released in M36.

In recognition of the varying manufacturing processes developed under the GREEN-LOOP project, which stem from the diverse types of products developed, IDE and AIMEN (as leader of tasks T2.2 and T2.3 respectively) have adhered to a standardized **methodology outlined in section 2** for every phase of the tasks. This methodology encompasses the following steps: gathering process data via questionnaires, illustrating the process steps in Process Flow Diagrams (PFDs), computing the inventory rate equations, and conducting the results analysis. This approach ensures consistency and comparability across the different process developments within the project. Regarding the Life Cycle Assessment (LCA) and Life Cycle Costing (LCC) evaluations, AIMEN adhered to established standards, specifically, the LCA was conducted in accordance with ISO 14040, while the LCC followed the UNE-EN 60300 guidelines.

The energy and exergy analysis for the manufacturing processes have been successfully conducted up to the current stage of the project. These evaluations offer valuable information regarding the energy consumption patterns and have enhanced the comprehension of the physical processes and mechanisms characterizing each step. Also, the exergy analysis has helped to gain understanding on the irreversibilities and energy losses that take place throughout the various stages of the processes, which contributes significantly to achieving the goals set for this task. LCA and LCC assessments have likewise been concluded with success. They have been instrumental in determining the key environmental impacts and associated costs. This analysis is crucial for understanding the broader implications of the manufacturing processes and for guiding strategic decisions aimed at sustainability and cost-efficiency, thereby aligning with the objectives of this task.

Furthermore, the tasks will continue until M36, to ensure the continuity of the work developed so far and support project partners with the upscaling of their manufacturing process. The energy and exergy analyses will place a special emphasis on identifying potential improvements and quantifying and understanding energy losses. LCA and LCC will incorporate data pertinent to industrial relevance, as in this first Deliverable only the raw materials and resources have been taken into account. Consequently, **Deliverable D2.3 – ‘Energy, Exergy, LCA, SLCA, and LCC Assessments**’ will be submitted at the project's conclusion (M36). This document will provide a refined analysis of the upscaled manufacturing processes evaluated during the second phase of the project.

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Nomenclature

Abbreviations and acronyms

AP	Acidification Potential
BoM	Bill of Materials
BRP	Bio-rubber panel
CE	Circular Economy
CFC-11	Clorofluorocarbon-11
ChCl	Choline Chloride
CTUh	Comparative Toxic Unit for human health
CTUe	Comparative Toxic Unit for ecosystems
DR	Discount Rate
EoL	End-of-Life
EP	Eutrophication Potential
FU	Functional Unit
GA	Grant Agreement
GHG	Greenhouse Gases
GWP	Global Warning Potential
ILCD	International Reference Life Cycle Data System
IRR	Internal Rate of Return
LCA	Life Cycle Assessment
LCC	Life Cycle Costing
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LDPE	Low-Density Polyethylene
MBTS-75	2,2' - Dibenzothiazyl Disulfide
mPt	Milli point
NPV	Net Present Value
ODE	Ordinary Differential Equation
ODP	Ozone Depletion Potential
PHBH	Poly(3-hydroxybutyrate-co-3-hydroxyhexanoate)
PLA	Poly(lactic acid)
POFP	Photochemical Oxidant Formation Potential
RM	Raw Materials
sLCA	Social Life Cycle Assessment
SO	Specific Objective
SOM	Soil Organic Matter
SKU	Stockkeeping units
TIN	Nominal Interest Rate
TRL	Technology Readiness Level

VC	Value Chain
WP	Work package

Symbols

c	Speed [m/h]
C	Concentration [mol/L]
C_P	Heat capacity [J·kg/K]
E	Total Energy [J]
$\dot{E}$	Rate of Energy [J/s]
g	Gravity constant = 9.81 [m/s2]
h	Specific enthalpy [J/kg]
H	Enthalpy [J]
m	Mass [kg]
$\dot{m}$	Mass flow [kg/batch]
M	Molecular mass [g/mol]
$\dot{n}$	Molar flow [mol/batch]
N	Number of moles [mol]
r	Reaction rate [The units depend on the system]
R	Molar gas constant = 8.3145 [J/K·mol]
P	Pressure [kg/m·s2]
Q	Volumetric flow [m3/h]
$\dot{Q}$	Heat flow [kJ/h]
t	Time [s]
T	Temperature [K]
u	Internal energy per unit mass [J/kg]
v	Specific volume [m3/kg]
V	Volume [m3]
x	Mass fraction [-]
X	Exergy [J]
$\dot{X}$	Rate of exergy [J/h]
$\dot{W}$	Rate of work [J/h]
z	Height [m]

Greek letters

α	Stoichiometric coefficient [-]
β	Volumetric expansion coefficient [-]
γ	Phase 1 of a component
Δ	Increment [-]
ε	Molar extent of the reaction [-]
η	Efficiency

λ	Enthalpy of phase change [J/kg]
ρ	Density [kg/m^3]
σ	Phase 2 of a component
ψ	Flow of exergy associated to a material stream [J/kg]

Subscripts

des	Destroyed
dis	Subindex for heat dissipated to the environment
flow	Flow
el	Electrical
gen	Generated
i	Material component / Chemical species
in	Inlet
j	Reaction number
k	Stream
out	Outlet
shaft	Shaft
sys	system
0	Ambient or “dead state”
F	Final
ref	Reference
R	Reaction
T	Total
Th	Thermal
P	Subscript to denote work associated to material streams
X	Exergetic

Superscripts

0	Standard
Tref	Evaluated at the reference temperature

1. Introduction

1.1. Purpose of this document

The purpose of this document is to compile the thermo-economic and environmental analysis linked to tasks T2.2 - *Energy and Exergy analysis of the systems* and T2.3 - *Tools and methodology for LCA, LCC, and Social LCA assessments* up to M22 of the project, encompassing the developments of the manufacturing process in the GREEN-LOOP’s value chains: bio-rubber, bioplastic and wood composites.

To this end, the document is divided in several sections pertaining the methodology followed through both analyses, the development of the equations and models for each value chain and a joint analysis of results for each manufacturing process, shedding light on possible improvements in the future upscale of the biomaterials manufacture up to TRL6.

1.2. Objectives

The main objectives of this deliverable are linked to the 1st Specific Objective (SO1) of the project “*to enhance green and smart features of manufacture*”, concretely to SO1.2 “*to increase the energy efficiency of the target production and manufacture processes*” and SO1.3 “Reduction of CO_2 emissions and resource utilisation”. Although the achievement of these objectives is directly related to the development of activities in WP3 to WP6, the analyses developed within WP2 aim to support the development and fine-tuning of these processes during their upscaling up to TRL6.

Furthermore, as included in the task’s description, both analyses will be performed at two phases: one at lab scale (compiling data from WP3 to WP5) and the other during the upscaling of the manufacturing, assessing then the final costs of products and including industrially relevant data. Among the main KPIs obtained during this 1st phase will be the irreversibility of the manufacturing process in terms of quality and quantity (thanks to the exergy analysis) and the main economic and environmental impacts of the processes (e.g., the GHG emissions).

1.3. Scope

On one hand, task T2.2 involves the energy and exergy analysis of the processes that comprise the 3 value chains developed in GREEN-LOOP, which are bio-rubber (NCC), bioplastic (LBRT) and wood composite (FHF) manufacturing. It is conducted with laboratory data, with the main limitation on the data available that partners can provide. To circumvent that, heuristics and data from literature have been consulted when necessary. Furthermore, in the final deliverable D2.3 the final exergy costs of the products manufacture will be assessed to support the upscaling of the process beyond the scope of the project. On the other hand, task T2.3 has the framework to carry out an LCA, an LCC and an sLCA for those 3 value chains represented in the GREEN-LOOP project. In this intermediate deliverable, we will focus exclusively on the environmental and economic analysis. This approach is taken because the scope of laboratory data currently available does not allow for a comprehensive sLCA. The limited scale and controlled conditions of the laboratory setting do not provide a sufficiently broad societal perspective to inform a representative sLCA at this stage. However, the laboratory environment can be considered as a microcosm of society. The societal analysis will be carried out in future stages when more extensive and diverse data can be collected to ensure a more accurate and meaningful assessment.

These analyses will be further developed based on the subsequent activities of WP2, and the complete final results will be subject of Deliverable D2.3 at the end of the project (M36). Conducting this joint preliminary analysis has a number of purposes for the development of the project, such as identifying hot spots for technical partners to work on, or selecting certain raw materials that are more environmentally friendly than others, identifying the main energy inefficiencies of the manufacturing process, etc.

2. Methodology

2.1. System definition

For the definition of each system to be analysed, firstly all respective WPL for each value chain (WP3/NCC Bio-rubber; WP4/LBRT/Bioplastic; WP5/FHF/Wood composites) have been contacted and requested information to better understand their manufacturing processes developed within GREEN-LOOP and create a series of process flow diagrams (PFDs) to support the development of inventory rate equations and the identification of inputs and outputs.

The PFDs follow the following structure:

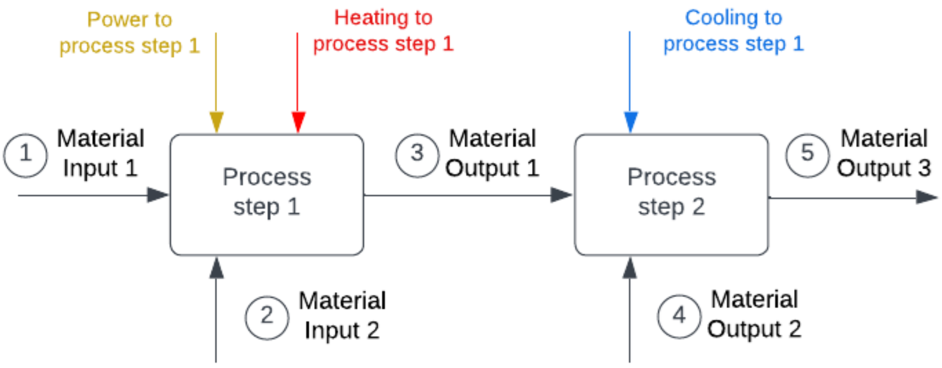

Figure 1. Example of a hypothetical PFD following the structure developed in T2.2

Once the PFDs for each manufacturing process were created, IDE collaborated with the responsible partners in the consortium to validate them. This served as the foundation for developing a questionnaire for each manufacturing process. The questionnaire requested project partners to provide information on mass flows, mass compositions, reaction kinetics (if applicable), energy consumption, and heating and cooling requirements, among other details.

Afterwards, IDE contacted the respective WPL again to verify and improve the data, resolving any possible deviations or minor inconsistencies that were found. Once the questionnaires have been validated, the process of developing the energy and exergy balances can begin. Any missing information will be addressed by utilising literature data and heuristics as needed.

The complete iterative data gathering protocol for task T2.2 is described in the following figure:

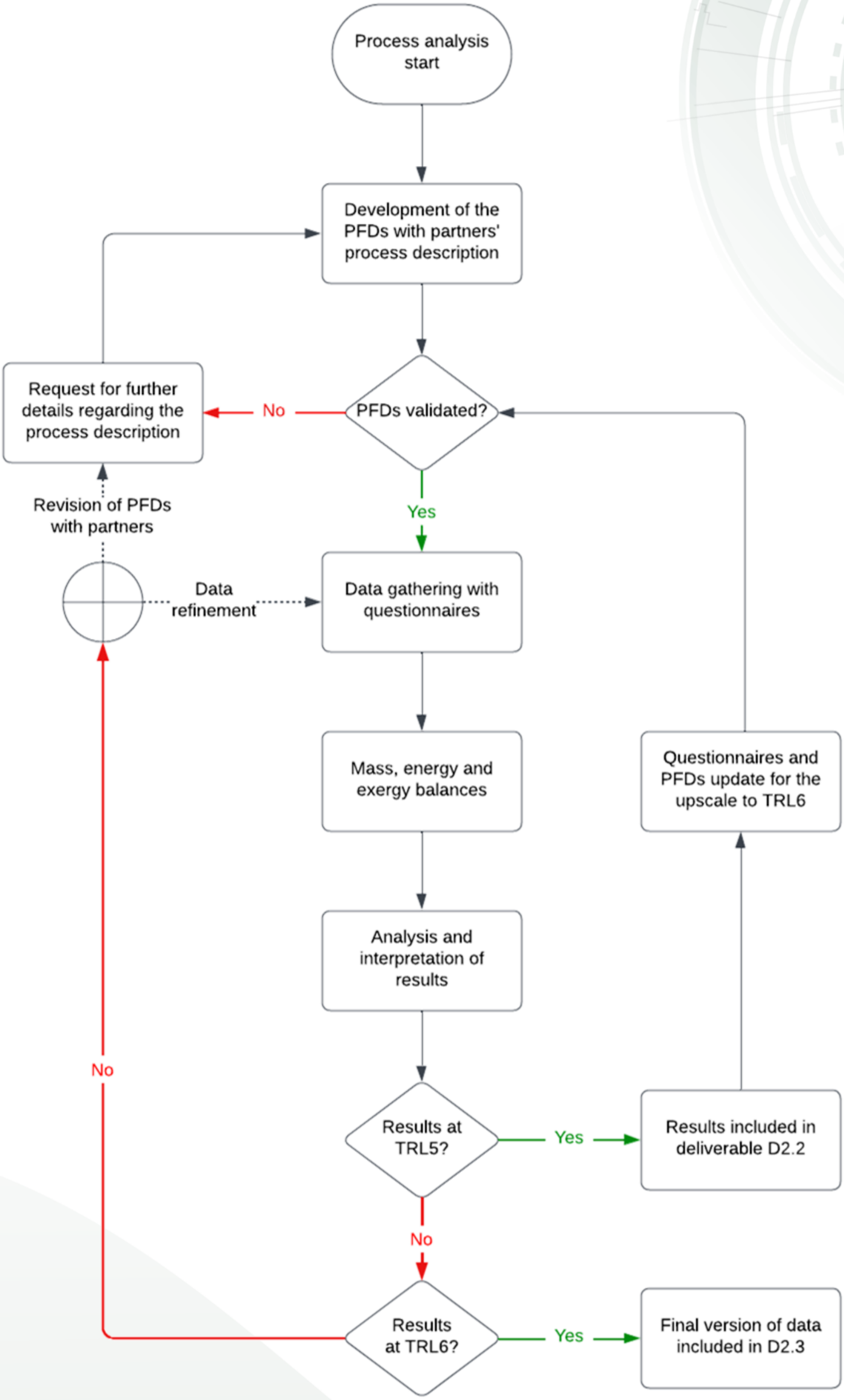

Figure 2. Data gathering protocol used in task T2.2

2.2. Energy and exergy analysis

To perform mass, energy and exergy analysis of industrial processes, it is necessary to develop inventory rate equations for each of the process steps in the system (1) using the laws of conservation of mass, energy or momentum and additional physics laws if necessary.

All inventory rate equations are comprised of the following terms:

$$\begin{pmatrix}Rate\ of\\ input\ of\ i\end{pmatrix}-\begin{pmatrix}Rate\ of\\ output\ of\ i\end{pmatrix}+\begin{pmatrix}Rate\ of\\ generation\ of\ i\end{pmatrix}=\begin{pmatrix}Rate\ of\\ accumulation\ of\ i\end{pmatrix} \qquad (1)$$

Whereas “i” represents the variables that is being analysed, usually its mass, energy, exergy, or momentum. To define and solve the equations, several aspects of the manufacturing processes developed within GREEN-LOOP must be assessed with these next steps:

1) Definition of the systems, including components and limits, provided by the manufacturing partners.

2) List the assumptions used for the analysis: in order to perform the manufacturing system evaluation, the process is represented to a mathematically simple form through reasonable assumptions to enable a faster analysis.

3) Develop the proper inventory rate equations for each basic element in the system.

4) Use empirical correlations if necessary to evaluate transfer coefficients if they are not available.

5) Solve the algebraic and differential equations depending on the assumptions made for the system and using the initial conditions for the differential equations provided by manufacturing partners whenever necessary.

After all the inventory rates equations have been solved in a process, the analysis of mass flows and energy flows can be performed and represented in a Sankey diagram, which serves as a powerful visual tool not only by shedding light on any possible enhancements of the process, but also quantifying where it would be more efficient to do so.

2.2.1. Heuristics followed during the analysis

In order to facilitate the analysis of the systems at the current TRL and scale (lab-scale/pilot plant), the following assumptions have been considered following the usual standards in process engineering [1]:

- The total enthalpy of a system cannot be measured directly because the internal energy contains components that are unknown, not easily accessible, or are not of interest for the thermodynamic problem at hand. Therefore, when performing and energy analysis is paramount to define a reference temperature T_{ref} and state of matter to properly assess changes in the energy of a system.

- Although the specific heat capacities of components and mixtures varies with temperature, at small changes of temperature a mean value between both range values can be used without significant deviations (e.g., in the designing of heat exchangers).

- Considering the definition of specific enthalpy:

$$dh = C_P dT + v(1 - \beta T)dP \qquad (2)$$

where h is the specific enthalpy, C_P is the specific heat capacity at constant pressure, T is the temperature, v is the specific volume, β is the volumetric expansion coefficient and P is the pressure. β is a difficult parameter to assess due to its definition:

$$\beta = \frac{1}{v}\left(\frac{\partial v}{\partial T}\right)_P = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_P \qquad (3)$$

Noting that:

$$\beta = \begin{cases} 0 & for\ an\ incompresible\ fluid \\ 1/T & for\ an\ ideal\ gas \end{cases}$$

At low and moderate pressures (< 10 bar), gases can be considered to be “ideal”, resulting in the following simplification:

$$\begin{cases} v(1 - 0 \cdot T)dP = vdP \ll C_P dT & for\ an\ incompresible\ fluid \\ v\left(1 - \frac{1}{T} \cdot T\right)dP = 0 & for\ an\ ideal\ gas \end{cases}$$

Therefore, considering low temperature increments and $h|^{Tref} = 0$:

$$\int_{Tref}^{T} dh = C_P \int_{Tref}^{T} dT \quad \therefore \quad h = C_P(T - T_{ref}) \qquad (4)$$

All the processes analysed here are considered as unsteady state without gradients within each phase, so the resulting macroscopic balances are ordinary differential equations in time. In the case that there is not accumulation of any property with time within the boundaries of the system evaluated, the macroscopic inventory rate equations are formed by algebraic equations.

Furthermore, considering that some of the process parameters are unknown to project partners due to being information only accessible to manufacturers (e.g. the efficiency of a motor of a specific potency), literature have been consulted when necessary, implementing the following set of heuristics common across process engineering:

- Energy efficiency of heating systems that are not fully detailed by each of the respective value chain owners is considered as 85% [2].
- As well as heating systems, the energy efficiency of cooling systems is assumed to be 70% [3].
- Energy efficiency of evaporator and compressor systems is considered as 70% in both cases [4].
- Every device driven by a motor (such as power supply devices) is assumed to have an energy efficiency of 85% [5].
- Energy efficiency of pumps is estimated to be 90% of the power required [4].

2.2.2. Inventory rate equations development

2.2.2.1. Mass balances

In this section of the document the development of the inventory rate equations for mass and energy balances is detailed. Considering the definition of $\dot{m}_i$ as mass flow of rates of species “i”, the following equivalences can be developed to express flow rates of a species “i” in terms of concentration and number of moles of that species:

$$\dot{m}_i = \rho_i Q_i = \frac{C_i}{M_i} Q_i \qquad (5)$$

$$\dot{n}_i = C_i Q_i \qquad (6)$$

Where ρ_i is the density of species; C_i is the molar concentration; M_i is the molecular weight; $\dot{n}_i$ is the molar flow and Q_i represents the volumetric flow of a species “i” in the system. The following table shows the most common sets of units used for each variable in the international system of units (SI):

Table 1. Units in the SI for the variables used to represent flows of species

Variable	Name	Units in the SI
$\dot{m}_i$	Mass flow of “i” species	kg/s
Q_i	Volumetric flow of “i” species	m^3/s
$\dot{n}_i$	Molar flow of “i” species	mol/s
C_i	Molar concentration of “i” species	mol/m^3
M_i	Molecular mass of “i” species	kg/mol
ρ_i	Density of “i” species	kg/m^3

It is important to note that although SI units are the most common across variables, in order to facilitate the calculation of results, unit conversions are used (e.g., the use of molecular weight in g/mol instead of kg/mol). Therefore, following the conservation of mass of the ith chemical species under unsteady-state process can be expressed as [1]:

$$\begin{pmatrix} Rate\ of\ mass \\ of\ i\ in \end{pmatrix} - \begin{pmatrix} Rate\ of\ mass \\ of\ i\ out \end{pmatrix} + \begin{pmatrix} Rate\ of \\ generation\ of\ mass\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ accumulation\ of mass\ of\ i \end{pmatrix} \qquad (7)$$

The mass of “i” may enter or leave the system by two means:

i. by inlet or outlet streams (represented as $(\dot{m}_i)_{in}$ and $(\dot{m}_i)_{out}$ respectively)
ii. by exchange of mass between the system and its surroundings through the boundaries of the system, i.e., interphase mass transfer (represented as $(\dot{m}_i)_{int}$). In closed system without several phases, the interphase mass transfer rate has a value of 0.

Furthermore, $(\dot{m}_i)_{in}$ and $(\dot{m}_i)_{out}$ can be expressed as the sum of all the mass flows entering and exiting the system respectively with the following formula:

$$(\dot{m}_i)_{in} = \sum_k (\dot{m}_i)_{k,in} \quad \therefore \quad (\dot{m}_i)_{out} = \sum_k (\dot{m}_i)_{k,out} \qquad (8)$$

Where “k” represents a material steam entering or exiting the system evaluated. If the following system boundaries can be considered:

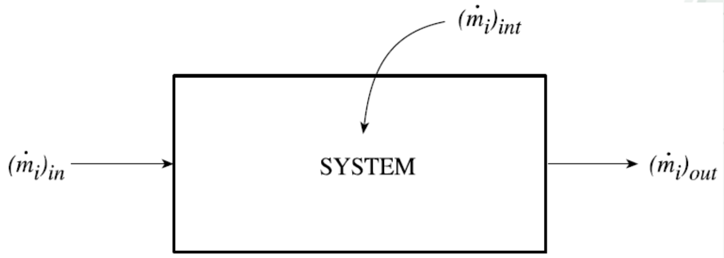

Figure 3. Unsteady-state flow system with fixed boundaries [1]

The following general inventory equation for mass balances can be developed using mass units:

$$\sum_k (\dot{m}_i)_{k,in} - \sum_k (\dot{m}_i)_{k,out} + V_{sys} M_i \sum_j \alpha_{ij} r_j = \frac{d(m_i)_{sys}}{dt} \qquad (9)$$

If molar units are used:

$$\sum_k (\dot{n}_i)_{k,in} - \sum_k (\dot{n}_i)_{k,out} + V_{sys} \sum_j \alpha_{ij} r_j = \frac{d(n_i)_{sys}}{dt} \qquad (10)$$

Where V_{sys} is the volume of the system considered; α_{ij} is the stoichiometric coefficient for species “i” in the chemical reaction “j” , r_j represents the reaction rate of reaction “j”, that is, the speed of which the species “i” involved in the reaction are consumed or produced which may or not may be dependent of time, expressed as “t”.

The expression of reaction rates for each specific reaction is dependent on the system evaluated (type of chemical species reacting, the physical medium in which the reaction is taking place, the type of catalyst used and the physical mechanism, among others) and can be expressed using several types of kinetic models (also known as kinetic equations), such as Power-Law models, Langmuir–Hinshelwood-Hougen-Watson, Eley-Rideal and Michaelis–Menten among others, although specific system such as polymer system require the use of different models.

In order to solve the balances, the partners involved in the development of GREEN-LOOP biomaterials have been requested to provide the reaction kinetics and kinetic equations for the system. Where providing that information has not been possible, literature data or their own know-how has been applied.

If there are no chemical reactions in the system (thus the rate of generation of species “i” is 0), the inventory rate equation can be expressed as:

$$\begin{pmatrix} Rate\ of \\ generation\ of\ i \end{pmatrix} = V_{sys} \sum_j \alpha_{ij} r_j = 0 \quad \therefore \quad \sum_k (\dot{m}_i)_{k,in} - \sum_k (\dot{m}_i)_{k,out} = \frac{d(m_i)_{sys}}{dt} \qquad (11)$$

Furthermore, in the case of closed systems with chemical reactions (therefore the rate of generation of “i” being different from 0), the following equation can be obtained:

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix} = 0 \quad \therefore \quad V_{sys} \sum_j \alpha_{ij} r_j = \frac{d(n_i)_{sys}}{dt} \qquad (12)$$

Rearranging the terms of the previous equation:

$$\sum_j \alpha_{ij} r_j = \frac{1}{V_{sys}} \cdot \frac{d(n_i)_{sys}}{dt} = \frac{d(C_i)_{sys}}{dt} \qquad (13)$$

Where C_i represents the concentration of species “i” in the system. Finally, if the system operates following a steady state (therefore no dependency with time of the process parameters included), the inventory rate equation can be expressed as:

$$\begin{pmatrix} Rate\ of \\ accumulation\ of\ i \end{pmatrix} = \frac{d(m_i)_{sys}}{dt} = 0 \quad \therefore \quad \sum_k (\dot{m}_i)_{k,in} - \sum_k (\dot{m}_i)_{k,out} + V_{sys} M_i \sum_j \alpha_{ij} r_j = 0 \qquad (14)$$

2.2.2.2. Energy balances

Following the development of the inventory rate equations for the mass balances, a similar approach has been proposed. Considering a system with similar boundaries to the one outline in, a similar structure can be developed for the energy balances adapting **equation 1**:

$$\begin{pmatrix} Rate\ of \\ energy\ input \end{pmatrix} - \begin{pmatrix} Rate\ of \\ energy\ output \end{pmatrix} + \begin{pmatrix} Rate\ of \\ energy\ generation \end{pmatrix} = \begin{pmatrix} Rate\ of \\ energy\ accumulation \end{pmatrix} \qquad (15)$$

Energy may enter or leave the system by the following means [1]:

i. by inlet and/or outlet streams (represented as $\dot{E}_{in}$ and $\dot{E}_{out}$ respectively)
ii. by exchange of energy between the system and its surroundings through the boundaries of the system in the form of heat and work (represented as $\dot{Q}_{int}$ and $\dot{W}$ respectively). For the purposes of sign criteria, $\dot{Q}_{int}$ and $\dot{W}$ will be considered positive when energy is added to the system or work is done on the system respectively.

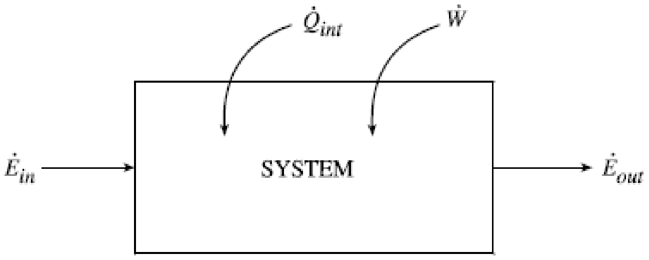

Figure 4. Unsteady-state flow system exchanging energy with the surroundings [1]

For the correct energy analysis of systems, it is mandatory to define a reference temperature T_{ref} and a phase of reference to account for enthalpy changes. The most common units for the rates of energy are J/s, W, kg·m^2/s^3, N·m/s or kcal/s among others. Following the sign criteria mentioned above, the elements of the inventory rate equation can be defined:

$$\begin{pmatrix} Rate\ of \\ energy\ input \end{pmatrix} = \dot{E}_{in} + \dot{Q}_{int} + \dot{W} = \sum_k (\dot{m}_k)_{in} \cdot \left(u_k + g z_k + \frac{{c_k}^2}{2} \right)_{in} + \dot{Q}_{int} + \dot{W} \qquad (16)$$

$$\begin{pmatrix} Rate\ of \\ energy\ output \end{pmatrix} = \dot{E}_{out} = \sum_k (\dot{m}_k)_{out} \cdot \left(u_k + g z_k + \frac{{c_k}^2}{2} \right)_{out} \qquad (17)$$

Where $\dot{E}_{in}$ represents the rate of energy entering the system, $\dot{E}_{out}$ represents the rate of energy exiting the system, $\dot{Q}_{int}$ the heat transfer rate, $\dot{W}$ the rate of work, u_k the internal energy per unit mass of a material steam, g the gravity constant (9.81 m/s^2), z_k the height of a material stream and c_k the speed of a material

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steam. The rate of work done on the system by the surroundings is given by three contributions: work associated with the expansion or compression of the system boundaries, shaft work and flow work:

$$\dot{W} = -P_{sys}\frac{dV_{sys}}{dt} + \dot{W}_{shaft} + \dot{W}_{flow} = -P_{sys}\frac{dV_{sys}}{dt} + \dot{W}_{shaft} + \sum_{k}(\dot{m}_k PV_k)_{in} - \sum_{k}(\dot{m}_k PV_k)_{out} \qquad (18)$$

Where the 1st term $-P_{sys}\frac{dV_{sys}}{dt}$ represents the work associated with expansion or compression of the volume (V_{sys}) in the system boundaries, $\dot{W}_{shaft}$ is the work associated with mechanical shafts within the systems (such as the shaft of pumps, compressors and other industrial equipment), $\dot{W}_{flow}$ is the work associated with the flow of mass entering or exiting the system, P is the pressure and V is the volume associated to a material steam. If there are not significant changes on the total volume of the system or the system operates in a steady state, the work associated with expansion or compression of the system is considered negligible or 0 respectively.

Furthermore, $\dot{W}_{shaft}$ can be calculated through the energy consumption of the equipment and their energy efficiency following this formula:

$$\dot{W}_{shaft} = \sum(\eta_{el}\cdot\dot{W}_{el}) = \sum\left(\eta_{el}\cdot\frac{E_{el}}{t}\right) \qquad (19)$$

Where η_{el} is the electric efficiency of the motor, $\dot{W}_{el}$ and E_{el} represents the power and energy consumed by the equipment. Additionally, the heat interchanged outside of the system can be expressed as:

$$\dot{Q}_{int} = \sum(\eta_{Th}\cdot\dot{Q}_{Th}) + \dot{Q}_{dis} = \sum\left(\eta_{Th}\cdot\frac{E_{Th}}{t}\right) + \dot{Q}_{dis} \qquad (20)$$

Where η_{Th} is the thermal efficiency of the equipment providing heating or cooling, $\dot{Q}_{Th}$ and E_{Th} represents the power and energy provided by the equipment and $\dot{Q}_{dis}$ the heat transfer rate with the environment (e.g., thermal losses). The term of the rate of energy generation can be described with the following expression:

$$\begin{pmatrix} \text{Rate of} \\ \text{energy generation} \end{pmatrix} = \sum \Delta H_R^{Tref} = \sum_j(\Delta H_j^{Tref}\cdot r_j) \qquad (21)$$

Where r_j represents the reaction rate of reaction “j”, ΔH_j^{Tref} represents the enthalpy of reaction at a reference temperature per mol unit for a reaction “j”, and ΔH_R^{Tref} represents the enthalpy of reaction rate for a reaction “j”. Following the sign criteria:

$$\Delta H_j^{Tref} = \begin{cases} > 0 & for\ endothermic\ reactions\ (requiring\ energy) \\ < 0 & for\ exothermic\ reactions\ (releasing\ energy) \end{cases}$$

If there are not any chemical reactions in the system analysed or the summatory of enthalpy of reactions rates are negligible (that is, low reaction rates or small enthalpies of reactions):

$$\begin{pmatrix} \text{Rate of} \\ \text{energy generation} \end{pmatrix} = \sum \Delta H_R^{Tref} = \sum_j(\Delta H_j^{Tref}\cdot r_j) = 0 \qquad (22)$$

Lastly, the rate of energy accumulated can be expressed with the following equation:

$$\begin{pmatrix} \text{Rate of} \\ \text{energy accumulation} \end{pmatrix} = \frac{dE_{sys}}{dt} = \frac{d}{dt}\left[m\cdot\left(u + gz + \frac{c^2}{2}\right)\right]_{sys} \qquad (23)$$

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Where m represents the mass of the system. If equations 15 to 23 are combined, the full inventory equation can be expressed as:

$$\sum_k (\dot{m}_k)_{in} \cdot \left(u_k + gz_k + \frac{{c_k}^2}{2}\right)_{in} - \sum_k (\dot{m}_k)_{out} \cdot \left(u_k + gz_k + \frac{{c_k}^2}{2}\right)_{out} + \dot{Q}_{int} - P_{sys}\frac{dV_{sys}}{dt} + \dot{W}_{shaft} + \sum_k (\dot{m}_k PV_k)_{in} - \sum_k (\dot{m}_k PV_k)_{out} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = \frac{d}{dt}\left[m \cdot \left(u + gz + \frac{c^2}{2}\right)\right]_{sys} \qquad (24)$$

The specific enthalpy of a material stream "k" can be defined as the following:

$$h_k = u_k + PV_k \qquad (25)$$

Due to the difficulty of assessing the value of the internal energy of a material steam or a system and considering equation 2, the following equivalences can be developed:

- Process at constant pressure and no phase change:

$$h_k = (u_k + PV_k) = u_k + PV_k = C_{P,k}(T_k - T_{ref}) \qquad (26)$$

- Process at variable pressure and no phase change:

$$h_k = \begin{cases} C_{P,k}\left(T_k - T_{ref}\right) + v\left(P - P_{ref}\right); If\ P > 10\ bar & (27) \\ C_{P,k}\left(T_k - T_{ref}\right); If\ P < 10\ bar\ or\ if\ the\ fluid\ is\ a\ gas & (28) \end{cases}$$

- Process at constant pressure and phase change: in this case is necessary to account for both the sensible heat and the latent heat of phase change for each system. Systems with phase change are non-steady processes, with a typical variation in temperature as a function of time described in the next figure:

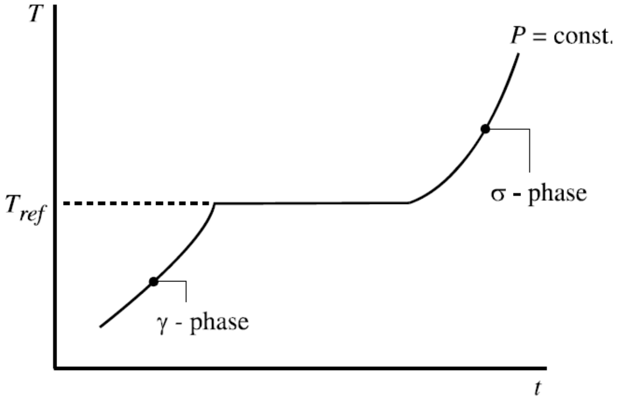

Figure 5. Temperature-time relationship as the substance transforms from the γ-phase to the σ-phase [1]

Considering the definition of specific enthalpy described in equation 2 and depending on the reference temperature used, several expressions can be obtained, for the purposes of simplifying the calculations, a T_{ref} lower than the T in which the material changes phases is selected, thus obtaining:

$$h_k = C_{P,k,\gamma} \cdot \left(T_{Phase\ Change} - T_{ref}\right) + \lambda + C_{P,k,\sigma} \cdot \left(T_k - T_{Phase\ Change}\right) \qquad (29)$$

Combining equation 23 and 24, the resulting general inventory equation for energy balances with no phase changes and operating at a constant pressure can be obtained:

$$\sum_k (\dot{m}_k)_{in} \cdot \left(h_k + gz_k + \frac{{c_k}^2}{2}\right)_{in} - \sum_k (\dot{m}_k)_{out} \cdot \left(h_k + gz_k + \frac{{c_k}^2}{2}\right)_{out} + \dot{Q}_{int} - P_{sys}\frac{dV_{sys}}{dt} + \dot{W}_{shaft}$$
$$+ \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = \frac{d}{dt}\left[m \cdot \left(u + gz + \frac{c^2}{2}\right)\right]_{sys} \qquad (30)$$

When the changes in the kinetic and potential energies between the inlet and outlet of the system as well as within the system are negligible [1]:

$$\sum_k (\dot{m}_k)_{in} \cdot \left(gz_k + \frac{{c_k}^2}{2}\right)_{in} = \sum_k (\dot{m}_k)_{out} \cdot \left(gz_k + \frac{{c_k}^2}{2}\right)_{out} \quad \therefore \quad \frac{d}{dt}\left[m \cdot \left(gz + \frac{c^2}{2}\right)\right]_{sys} = 0$$

$$\sum_k (\dot{m}_k \cdot h_k)_{in} - \sum_k (\dot{m}_k \cdot h_k)_{out} + \dot{Q}_{int} - P_{sys}\frac{dV_{sys}}{dt} + \dot{W}_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = \frac{d(m \cdot u)_{sys}}{dt} \qquad (31)$$

Finally, if the system is operating at a steady-state, equation 29 can be further simplified to:

$$\sum_k (\dot{m}_k \cdot h_k)_{in} - \sum_k (\dot{m}_k \cdot h_k)_{out} + \dot{Q}_{int} + \dot{W}_{shaft} = 0 \qquad (32)$$

The general equation can also be described in general terms, rather than rates. Not all the data related to the process times described in the following sections have been provided. Therefore, the equations used are expressed in general terms.

$$(Energy\ input) - (Energy\ output) + (Energy\ generation) = (Energy\ accumulation) \qquad (33)$$

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} - P_{sys}\Delta V_{sys} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = \Delta(m \cdot u)_{sys} \qquad (34)$$

The following table shows the most common sets of units used for each variable in the SI:

Table 2. Units in the SI for the variables used to represent energy balances

Variable	Name	Units in the SI
m_k	Mass of “k” species	kg
h_k	Specific enthalpy of “k” species	J/kg
Q_{int}	Heat exchange	J
W_{shaft}	Work	J
ΔH_j^{Tref}	Enthalpy of a reaction	J/kg

2.2.2.3. Exergy balances

Regarding exergy balances, a similar approach can be followed as with the mass and energy balances but considering the second law of thermodynamics (SLT). The nature of exergy is opposite to that of entropy, in which exergy can be destroyed but cannot be created [6].

Therefore, the exergy change of a system during a process is less than the exergy transfer by an amount equal to exergy destroyed within the system boundaries during the process [6]. Then, the following equation can be developed:

$$\begin{pmatrix} Rate\ of \\ exergy\ input \end{pmatrix} - \begin{pmatrix} Rate\ of \\ exergy\ output \end{pmatrix} + \begin{pmatrix} Rate\ of \\ exergy\ destruction \end{pmatrix} = \begin{pmatrix} Rate\ of \\ exergy\ change \end{pmatrix} \qquad (35)$$

$$\dot{X}_{in} - \dot{X}_{out} - \dot{X}_{destr} = \frac{dX_{sys}}{dt} \qquad (36)$$

Where $\dot{X}$ represent the exergy rate, and X_{sys} the total exergy of the system evaluated. The exergy balance can also be expressed with total amounts instead of rates, obtaining the following equation:

$$X_{in} - X_{out} - X_{destr} = \Delta X_{sys} \qquad (37)$$

Exergy (X) can be transferred into and out of a system by heat ($\dot{X}_Q$), mass flows ($\dot{X}_m$) or work made ($\dot{X}_W$), considering the following equivalences:

$$\dot{X}_Q = \left(1 - \frac{T_0}{T}\right) \cdot \dot{Q}_{int} \qquad (38)$$

$$\dot{X}_m = \dot{m}_k \psi = \dot{m}_k \cdot \left[(h_k - h_0) - T_0 \cdot (s_k - s_0) + g z_k + \frac{{c_k}^2}{2}\right] \qquad (39)$$

$$\dot{X}_W = \dot{W} - P_0 \frac{dV_{sys}}{dt} \qquad (40)$$

Entropy values are difficult to quantify, and depends on different variables, which makes impossible to find standard values in bibliography. The following estimation for entropy is used for solid and liquid compounds.

$$s_k = C_{P,k} \cdot ln \frac{T_k}{T_{ref}} \qquad (26)$$

Where ψ is the flow of exergy associated to a material stream, T_0 is the ambient temperature, s_0 represents the entropy of the system evaluated at ambient temperature (also called "dead state", the state of a system where it is in complete equilibrium with its surroundings, thus having no potential to do work).

Additional considerations can be made depending on the nature of the system:

- If the system is adiabatic $\dot{Q}_{int} = 0$, then $\dot{X}_Q = 0$.
- For closed systems (e.g., system where there are not any mass flows), $\dot{X}_m = 0$

Regarding the rate of energy destroyed (also called "irreversibility" of the system), it can be calculated with the following equation [6]:

$$\dot{X}_{destr} = T_0 \dot{S}_{gen} \geq 0 \qquad (41)$$

Furthermore, depending on the value obtained, process can be classified with the following classification:

$$\dot{X}_{destr} \begin{cases} > 0\,; Irreversible\ process \\ = 0\,; Reversible\ process \\ < 0\ Impossible\ process \end{cases}$$

Then, considering the principle of exergy destruction, the total of exergy destroyed cannot be negative, however, the change of type of exergy in a process can be positive or negative. Considering the sign criteria discussed in the previous section ($\dot{Q}_{int}$ and $\dot{W}$ will be considered positive when energy is added to the system or work is done on the system respectively). For a closed system, the total exergy balance can be expressed as:

$$X_{in} - X_{out} - X_{destr} = \Delta X_{sys} \qquad (42)$$

$$\sum\left(1-\frac{T_0}{T}\right)Q_{int} + [W - P_0(V_2 - V_1)] - T_0 S_{gen} = \Delta X_{sys} \qquad (43)$$

If expressed as a rate equation:

$$\sum\left(1-\frac{T_0}{T}\right)\dot{Q}_{int} + \left[W - P_0\frac{dV_{sys}}{dt}\right] - T_0\dot{S}_{gen} = \frac{dX_{sys}}{dt} \qquad (44)$$

Where, S_{gen} represent the total entropy generated in the system $\dot{S}_{gen}$ represents the rate of generation of entropy of the system. For an open system, both equations 41 and 42 can be adapted to the total and rate version of the balance respectively:

$$\sum\left(1-\frac{T_0}{T}\right)Q_{int} + [W - P_0(V_2 - V_1)] + \sum(m_k \cdot \psi)_{in} - \sum(m_k \cdot \psi)_{out} - T_0 S_{gen} = \Delta X_{sys} \qquad (45)$$

$$\sum\left(1-\frac{T_0}{T_k}\right)\dot{Q}_{int} + \left[\dot{W} - P_0\frac{dV_{sys}}{dt}\right] + \sum(\dot{m}_k \cdot \psi)_{in} - \sum(\dot{m}_k \cdot \psi)_{out} - T_0\dot{S}_{gen} = \frac{dX_{sys}}{dt} \qquad (46)$$

For steady state, the previous equation can be simplified to:

$$\left(\begin{matrix} Rate\ of \\ exergy\ change \end{matrix}\right) = 0$$

$$\sum\left(1-\frac{T_0}{T_k}\right)\dot{Q}_{int} + \left[\dot{W} - P_0\frac{dV_{sys}}{dt}\right] + \sum(\dot{m}_k \cdot \psi)_{in} - \sum(\dot{m}_k \cdot \psi)_{out} - T_0\dot{S}_{gen} = 0 \qquad (47)$$

Finally, a general definition of exergy efficiency (η_X) can be utilised:

$$\eta_X = \frac{Exergy\ obtained}{Exergy\ consumed} = 1 - \frac{T_0\dot{S}_{gen}}{Exergy\ consumed} \qquad (48)$$

For an open system, the total exergy balance can be expressed as follows:

$$\sum\left(1-\frac{T_0}{T}\right)Q_{int} + [W - P_0(V_2 - V_1)] + \sum(m_k \cdot \psi)_{in} - \sum(\mathrm{m}_k \cdot \psi)_{out} - T_0 S_{gen} = \Delta X_{sys} \qquad (49)$$

The following table shows the most common sets of units used for each variable in the international system of units (SI):

Table 3. Units in the SI for the variables used to represent exergy balances

Variable	Name	Units in the SI
m_k	Mass of "k" species	kg
ψ	Exergy exchange	J/kg
Q_{int}	Heat exchange	J
W	Work	J
S_{gen}	Generated entropy	J/K

2.3. Life Cycle Analysis

To develop the study regarding the environmental impacts for all the value chains (VCs) along the GREEN-LOOP Project, it has been proposed a Life Cycle Analysis (LCA), across the 3 fundamental pillars of sustainability: environment, economic and social.

The objective of this study is to assess the manufacturing of each use case based on the data obtained from the three involved value chains during the life of the Project in every technical Work Package (WP): bio-rubber panels (in WP3 context), bioplastic closures (WP4 conditions) and wood composites (from WP5 developments).

The Life Cycle Assessment (LCA) will measure the different environmental impacts of a product, process or system throughout its whole life cycle, from the extraction of Raw Materials (RM) until the End-of-Life (EoL). The goal of the assessment is to collect and analyse the inputs and outputs of the system to obtain the results as potential environmental impacts, to establish the strategies of reduction. The environmental impacts will be compared with the current manufacturing process of each bio-based process in development for this project.

The main idea of this tool is its holistic point of view, i.e. it is based on the fact that all properties of a system cannot be determined or explained only individually by the parts that compose it, an integration of all aspects involved is needed. That is why the whole life cycle of the system has to be taken into account. The elements involved in the LCA are usually defined as inputs/outputs:

- **Inputs:** Use of Raw Materials, parts or products; Transport; Electricity; Energy Requirements, etc., which are considered in each process/phase of the system.

- **Outputs:** Emissions to air, water and soil; Wastes and By-products that are considered in each process/phase of the system.

All these inputs/outputs are collected within a Life Cycle Inventory (LCI), and it is the phase of the LCA involves the collection and quantification of these items during their entire life cycle: the extraction of raw materials and the manufacturing of needed materials for the processing of components, the use phase of the final product and the recycling or final disposal/management. When the transport, the storage, distribution or other quite important activities, should be included in the analysis. The name of this scope of this kind of LCA is “Cradle-to-Grave”.

When the analysis does not take all the stages and stops when the product is on the market (just after de manufacturing step) is referred as “Cradle-to-Gate” scope.

Finally, when it is taken into consideration only the data of the manufacturing process, it is denominated “Gate-to-Gate” scope; on the other hand, when the output from the EoL system is evaluated and reuse it as raw material, then it will be a scope called “Cradle-to-Cradle”.

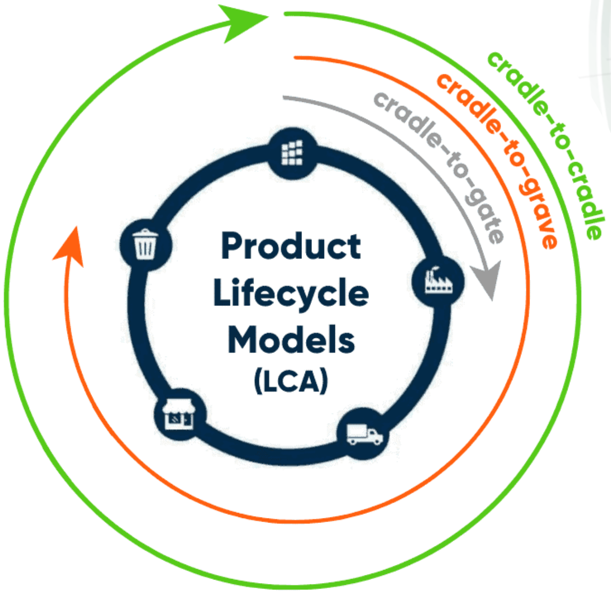

Figure 6. Different scopes for LCA [7]

The phase inside the LCA when happens the collection of all inputs/outputs are the basis for the subsequent analysis and assessment of the environmental effects related to the manufacturing of products. This summation of resources and emissions towards environmental and human damage is called Life Cycle Impact Assessment (LCIA). This LCIA refers to the steps that assess the type and extent of environmental impacts that may arise quantitatively based on data collected in the LCI.

The economic impacts (direct cost, indirect cost, …) related with a product, service or building will be evaluated across the Life Cycle Costing (LCC), from the conception of the idea until the end of its life cycle, taking into account all the phases of the life cycle.

In the design phase, together with the environmental analysis, a thorough knowledge of the costs involved in all the stages of the product's life cycle allows take decisions to be made that include economic items that would otherwise not be assigned to the system under study. The LCC facilitates the integration of the economic and environmental aspects as pillars and values of the GREEN-LOOP project, considered as a single system throughout its whole life cycle.

Therefore, LCC is not a business costing tool, but expresses the monetary value of an asset taking into account the internal costs associated with its life cycle. LCC quantifies the relationship between economic and environmental optimisation of the system under consideration to understand how economic activities affect environmental activities and vice versa. LCC is ideally suited for application to products and building components, providing cost savings and quantifying the economic value of the environmental improvements of these products and services.

After the environmental and economic pillars, the next one is social. This last impact analysis is developed with the social Life Cycle Assessment (sLCA). The social aspect will not have a solid development at this time in the Project, due to the fact that all the data evaluated for this deliverable are from a lab scale, and there is no point in developing and studying the impacts on society of a process that is still on a small laboratory scale. For this intermediate deliverable, social aspects have not been considered because the GREEN-LOOP Project is still at too early a stage (laboratory scale) to study whether the bio-based products manufactured during the GREEN-LOOP Project can generate impacts on society. As it was mentioned above, this analysis will be developed for the final deliverable (D2.3) at the end of the project in M36.

2.3.1. Methodology description

The following sub-sections explain the methodology used for the environmental and economic analyses. This explanation describes the standards followed, the different steps and the values obtained from the analyses.

2.3.1.1. LCA Methodology

ISO, the International Organisation for Standardisation, has established a framework for the standardisation of the LCA methodology, according to the ISO 14.040 family of standards:

- **UNE EN ISO 14.040:2006:** Environmental management. Life Cycle Analysis. Principles and reference framework [8].

- **UNE EN ISO 14.044:2006:** Environmental management. Life Cycle Analysis. Requirements and guidelines [9]. According to the standardisation carried out, four phases can be distinguished in an LCA study (as described in Figure 7):

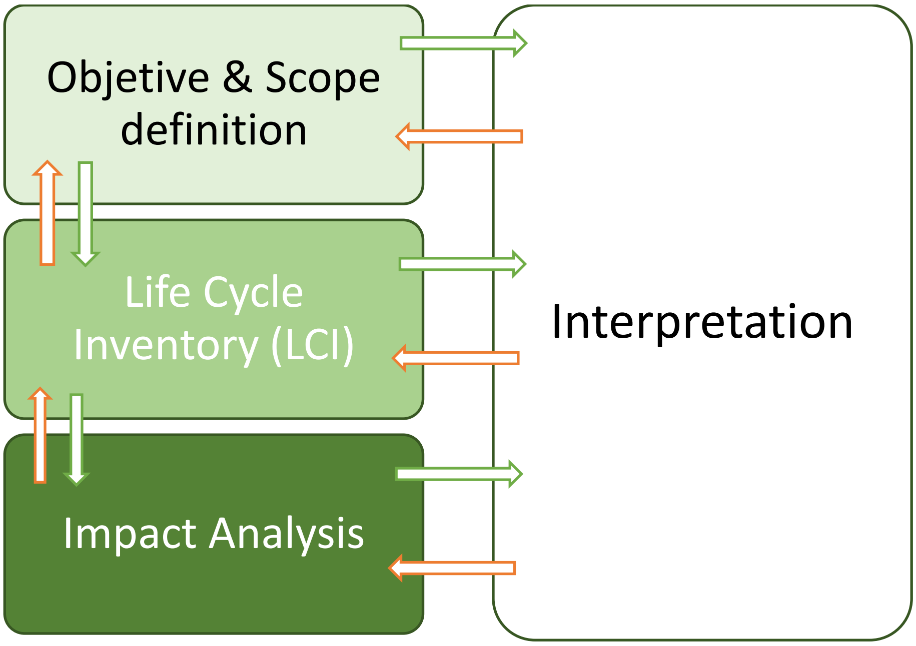

Figure 7. Steps of a LCA according to ISO 14.040

- ○ Definition of Objectives and Scope: Defines the objective and intended use of the study, as well as the scope according to the system boundaries, the functional unit and flows within the life cycle, the required quality of the data, and the technological and evaluation parameters.

- <u>Development of the Life Cycle Inventory (LCI)</u>: This is the phase of the LCA in which data is collected on the inputs and outputs for all processes of the product system.

- <u>Life Cycle Impact Assessment (LCIA)</u>: This is the phase of the LCA in which the inventory of inputs and outputs is transferred into indicators of potential environmental impacts on the environment, human health and natural resource availability.

- <u>Interpretation</u>: This is the phase of the LCA in which the results of the LCI and LCIA are interpreted according to the objective and scope initially set. In this phase, an analysis of the results is carried out and conclusions are drawn.

Life Cycle Impact Assessment (LCIA)

LCIA is the phase inside the LCA which understand and assess the approach and the magnitude of the different environmental impacts of the system. With this step it takes place the transformation of data collected into environmental results.

The first step in the LCIA is to select the environmental impact categories to be considered in the study. These categories represent the environmental impacts of interest to which the results of the LCIA will be assigned. In other words, the environmental impacts for which results are desired. There are several environmental impact categories and the choice for the LCA will depend on the objective of the study, the target audience and the level of precision of the results required. Some of the most common that are also included in the International Reference Life Cycle Data System (ILCD) methodology used in this study, are discussed in Table 4. Some aspects, as recyclability, reuse, refurbish, or waste reduction, will be calculated and commented during the final update of this deliverable at the end of the project in M36.

Table 4. Environmental Impact categories considered in LCA

Environmental impact category		Reference unit	Characterisation factor
Global warming	A phenomenon observed in temperature measurements that shows on average an increase in the temperature of the Earth's atmosphere and oceans over the last decades	kg CO_2 eq	Global Warning Potential (GWP)
Consumption of raw materials	Consumption of materials extracted from nature.	kg Sb eq	Quantity Consumed
Consumption of Energy Resources	Energy consumed in obtaining raw materials, manufacturing, distribution, use and end of life of the item under analysis.	MJ	Quantity Consumed
Ozone depletion	Negative effects on the solar ultraviolet radiation protection capacity of the atmospheric ozone layer.	kg CFC-11 eq	Ozone Depletion Potential (ODP)
Formation of photochemical oxidants	Formation of the precursors that give rise to photochemical pollution. Sunlight strikes these precursors, causing the formation of a series of	kg C_2H_4 eq	Photochemical Oxidant Formation Potential (PFOF)

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Environmental impact category		Reference unit	Characterisation factor
	compounds known as photochemical oxidants (ozone-O3 is the most important due to its abundance and toxicity).		
Eutrophication	Excessive growth of algal populations caused by artificial enrichment of river and reservoir waters as a result of massive use of fertilisers and detergents leading to high oxygen consumption in the water.	kg de NO_3 eq	Eutrophication Potential (EP)
Acidification	Loss of the neutralising capacity of soil and water, resulting from the return of sulphur and nitrogen oxides discharged into the atmosphere to the earth's surface in the form of acids.	kg SO_2 eq	Acidification Potential (AP)
Ecotoxicity	Category relating to toxic impacts affecting an ecosystem, which are harmful to different species, and which change the structure and function of the ecosystem.	kg 1,4-DB eq	Freshwater ecotoxicity / Marine ecotoxicity / Terrestrial ecotoxicity
Human ecotoxicity	Category for harmful effects on human health due to the uptake of toxic substances through inhalation of air, ingestion of food or water, or penetration through the skin, in so far as they are related to cancer and non-cancer effects.	kg 1,4-DB eq	Human ecotoxicity

In the classification stage, each data from LCI is assigned to each impact category. If a substance/product is a contributor to more than one impact category, it should be considered in all impact categories.

International Reference Life Cycle Data System (ILCD)

ISO 14040 [8] and 14044 [9] provide the indispensable framework for LCA. However, this framework leaves the individual practitioner with several options, which can affect the legitimacy of the results of an LCA study. While flexibility is essential to respond to the wide variety of issues being addressed, further guidance is needed to support consistency and quality assurance. Therefore, the International Reference Life Cycle Data System (ILCD) [10] has been developed to provide guidance for consistent and quality assured LCA data and studies.

The development of the ILCD has been coordinated by the European Commission and has been carried out through an extensive international consultation process with experts, stakeholders and the public. LCIA methods exist for the midpoint level and for the endpoint level, and for both in integrated LCIA methodologies. In general, at the mid-point level a larger number of impact categories are differentiated (typically around 10) and the results are more accurate and precise compared to the three protection areas at the endpoint level that are commonly used for endpoint assessments.

The following impact categories at mid-point level and Protection Areas will be checked by default for their relevance to the study and related LCIA methods will be identified for use in the life cycle impact assessment phase of the LCA, Table 5: Climate change, Ozone depletion (stratospheric), Human toxicity, Respiratory inorganics, Ionizing radiation, Photochemical ozone formation (ground level), Acidification (land and water), Eutrophication (land and water), Ecotoxicity, Land use, Resource depletion (minerals, fossil and renewable energy resources, water). A short description of most of them are already in Table 5.

Table 5. Midpoint impact categories considered in ILCD methodology

Impact category	**Indicator**
Climate change	Global Warming Protection (GWP 100) in CO_2 equivalent
Ozone depletion	Ozone Depletion Potential (ODP 100) in clorofluorocarbon-11 equivalents (CFC-11)
Human toxicity, non-cancer effects	Comparative Toxic Unit for human health (CTUh)
Human toxicity, cancer effects	Comparative Toxic Unit for human health (CTUh)
Particulate matter	Particulate matter, medium diameter 2.5E-06 µm (PM2.5)
Ionizing radiation HH	Ionizing Radiation Potentials (Uranium 235)
Ionizing radiation E (interim)	Photochemical ozone creation potential in Ethylene equivalent (C_2H_4)
Photochemical ozone formation	Mol hydrogen equivalent (H^+)
Acidification	Mol hydrogen equivalent (H^+)
Terrestrial eutrophication	Mol hydrogen equivalent (H^+)
Freshwater eutrophication	Comparative Toxic Unit for ecosystems (CTUe)
Marine eutrophication	Soil Organic Matter (SOM), in (kg C/m^2/a).
Freshwater ecotoxicity	Water consumption equivalent (m^3)
Land use	Scarcity [Production/ (Ultimate Reserve)2] compare with antimony (Sb)

This is done using characterisation factors for each substance, which represent its contribution to a given impact category relative to the reference substance in that category. Each substance is multiplied by its respective characterisation factor. This gives equivalent unit values that can be summed to measure the contribution of substances to that impact category.

In addition to the mandatory steps to be performed in the LCIA, there are optional steps that can be taken depending on the objective and intended scope. These are as follows:

- **Normalisation:** Conversion of the characterisation results to global neutral units, dividing each by a normalisation factor. These factors represent the degree of contribution of each impact category to the local environmental problem.
- **Grouping:** Classification of impact categories into other groups encompassing impact categories with similar effects.
- **Weighting:** Conversion of the results of the characterised values into a common and summable unit (in case the methodology includes a normalisation, from the normalised values), by multiplying them by their weighting factor. They are then summed to obtain a single total score for the environmental impact of the system.

2.3.1.2. LCC Methodology

For the development of the LCC, AIMEN has followed the standard **UNE-EN 60300** [11]. This standard is oriented towards a LCC related with reliability, as operation, safety, maintainability, maintenance, support, requirements, etc., although it is the only published standard for the product and was therefore chosen for the development of this LCC. There are more well-known global standards to the development of the LCC, as UNE-EN 15643-4:2012, UNE-EN 16627:2016 or ISO 15686-5:2017, but all of them are not viable for use under the GREEN-LOOP project because are aimed to life cycle costing for buildings.

The performance for calculation of LCC has the following steps listed in the standard UNE-EN 60300, mentioned above:

- Quantify the differences in product performance, availability, and other relevant constraints between each of the alternatives considered, unless these differences are directly reflected in the results of the LCC model.
    - Data collection of all basic cost elements of the LCC model for all product options.
    - Perform LCC analysis of product operational scenarios defined in the analysis plan.
    - Identification of optimal support scenarios.
    - Review of baseline data and results of the LCC model to determine which cost elements have the most significant impact on the analysis.
- Quantify the differences in product performance, availability and other relevant constraints between the alternatives considered, unless these differences are directly reflected in the results of the LCC model.

- Classify and summarise the results of the LCC model according to a logical grouping (recurring or non-recurring costs, acquisition, ownership or disposal costs, etc.) that may be relevant to the users of the analysis results.

- Perform sensitivity analyses to examine the impact of assumptions and uncertainties about cost elements on the results of the LCC model, paying particular attention to key cost drivers and assumptions about product usage and the time value of money.

- Review the LCC results and compare them with the objectives defined in the analysis plan to ensure that all objectives have been met and that sufficient information has been provided to support the required decision.

Terminology

In order to develop the LCC, several values related to economy have to be calculated and used in this analysis, which are defined below:

- **NPV (Net Present Value):** It is the sum of discounted future cash flows (i.e., discounted at a discount rate), both costs and revenues.

- **Cash Flows:** Are the (negative) expenses and (positive) revenues at a given time.

- **Discount Rate (DR):** It is the interest rate that has been adopted in order to be able to express the monetary values of the future in current values.

- **Internal Rate of Return (IRR):** The interest rate or return on an investment.

- **Interest Rate**: This is the amount paid in a time unit for each unit of capital invested.

- **Nominal Interest Rate (TIN)**: It is profitability obtained in a financial operation that is capitalised in a simple way, allowing for only the main capital. It is the opportunity cost that a bank's client has (profitability that he obtains) for not having the money. In this rate the inflation rate is not discounted.

- **Inflation**: It is the widespread and sustained increase in the prices of goods and services in a country over a period, usually one year

Assumptions and considerations in LCC analysis

Across the life of the GREEN-LOOP Project, the LCC will consider the main aspects that affect the costs of the bio-based components during their whole entire life, although in this case it was selected a “Cradle-to-Gate” scope, including only the manufacturing process, considering the raw materials purchased to develop the bio-based components. It has been considered:

- Raw materials (including the auxiliary).
- Direct manufacture costs: energy consumption and labour (hours).
- Indirect manufacture costs: equipment purchases, waste management and other costs (5% of direct cost).
- Manufacture profits: 7% of raw materials, direct and indirect manufacture costs.
- Environmental externalities.

Environmental externalities are the cost associated with the palliation of an affection achieved on the environment (i.e., the energy consumption causes a series of emissions that cause impacts on the environment). These costs have an impact on the global economy of the process, and to calculate the environmental externalities, a European method developed by CE Delft has been followed [12].

This method is comprised of five steps:

i) Updating monetary values of the endpoint categories on basis of literature, General SCBA Guidelines and Discount Rate Working Group,
ii) Updating the impact pathway analyses, which specify the relationship between emissions in the Netherlands and impacts on endpoints,
iii) Valuation of 15 pollutants on basis of inputs from the previous steps and literature,
iv) Allocation of those pollutants to midpoint impact categories in ReCiPe 2008,
v) Deriving weighted average value for damage to midpoint categories in order to calculate the damage cost for each substance characterised in ReCiPe 2008 and midpoint damage factors.

Environmental externalities will help to demonstrate that bio-based materials have the potential to be more environmentally friendly than traditional fossil-based materials, although environmental impacts must be carefully assessed through life cycle assessment (LCA) studies. In summary, while bio-based materials have environmental advantages, their LCAs must consider a wide range of impact categories, end-of-life scenarios, particulate pollution, and the unique challenges of emerging technologies. Standardized methods and more comprehensive modelling of environmental externalities are needed to fully assess the sustainability of bio-based materials.

2.3.2. Datasets and computational tools used

To conduct a Life Cycle Assessment (LCA) study, various datasets are essential for analysing the environmental impacts of products. These datasets provide crucial information on the life cycle of products, from raw materials to disposal. The large dataset size allowed the results to be broken down by product category, brand, and even individual stockkeeping units (SKUs). This granular analysis can help consumers make more informed purchasing decisions and guide companies on how to prioritize sustainability improvements in their product portfolios [13].

The study demonstrates the value of compiling comprehensive LCA datasets to assess the environmental performance of consumer products. However, challenges remain in terms of data collection, allocation between co-products, and interpreting the results. Ongoing efforts are needed to expand and improve LCA datasets to support evidence-based decision making [14].

Along the life of the GREEN-LOOP Project, Ecoinvent 3.10 will be the database used. This database is widely recognized as one of the largest, most consistent, and transparent databases for LCA, Ecoinvent contains over 18,000 unique datasets modelling human activities and processes, supporting a broad range of sustainability assessments [15]. Specifically, the database selected was Ecoinvent 3.10 [16], and the method selected for the calculation was ILCD, that includes the impact categories described in Table 5. For the assessment, the SimaPro 9.6 software, developed by Pré-Consultants, was used to calculate the different life cycle analyses.

For the development of the LCC, the datasets and the tools used will be the same as in the performance of the environmental one. The technical partners have provided mostly of the Market prices involved in the development of the LCC, as the equipment prices too.

The main way to obtain all the info is collecting data from technical partners with the inventories for each value chain. These inventories have as input the outputs from

i. **Task T2.1: Circular Economy, End of Life strategies and value chain assessment**; the Bill of Materials (BoM) developed in this task and during the Deliverable D2.1: GREEN-LOOP Circular Economy Evaluation, led by AXIA and GIG.

ii. **Task T2.2: Energy and Exergy analysis of the system**, led by IDE, will help to get all the information regarding the energy requirements (electricity, heat, cool…) related to the equipment use during the three different processes.

To perform these analyses will be needed to get some inputs related to manufacture, as kilograms and characterization of raw materials; the amount of electricity/heat and fuel/gas; the capacity and cost of the equipment; or the info for labour situation to use in LCC analysis. During the past months, the technical partners (from WP3, WP4 and WP5 – NCC, NIC, IRIS, LBRT, MYX, FHF) have been able to update these inventories while the accuracy of the processes was taking place. Due to the processes was suffering some changes and as the LCIs are a living documents, it was possible to update them at the same time as they were implemented at the process.

This way of continuously updating a living document by the technical partners is a form of validation of the data used in the analysis. When some data is missing, the protocol is to search some equivalent info in bibliography and literature, or to use some existing similar data. In the future, the main idea is to connect this work with the scale-up developed during the WP6: Upscale production and demonstration.

3. Technical analysis development

3.1. Energy and exergy analysis

3.1.1. Bio-rubber manufacture (WP3)

The bio-rubber value chain develop in WP3 involves three different processes. Apart from the general process in which rubber panels are processed, the bio-rubber value chain includes the production of lignin and the functionalisation of rubber that are used in the creation of rubber panels.

The PFDs (process flow diagrams) for each process are included in the next sections. It should be noted that the streams corresponding to the lignin extraction are denoted by the letter “a”, whereas the streams corresponding to the functionalisation of rubber to produce rubber crumb are denoted by the letter “b”. The streams calculated using experimental data are indicated by (E), while the ones derived from calculus are denoted by (C).

Mass balance

Lignin extraction

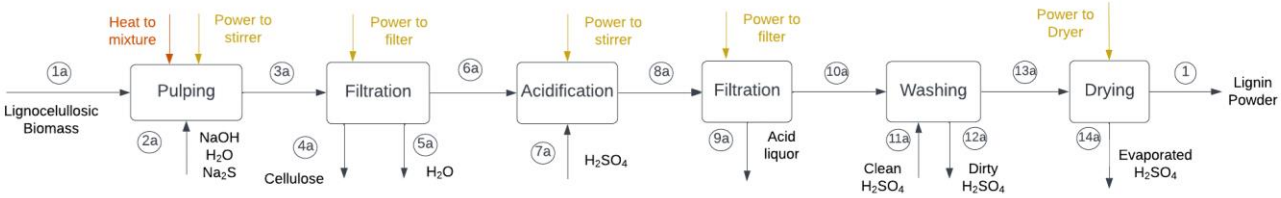

Figure 8. PFD for lignin extraction process.

As described in the methodology, in each step of the process, the following equation must be satisfied. The balances are expressed in grams per batch (g/batch).

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} - \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix} + \begin{pmatrix} Rate\ of \\ generation\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ accumulation\ of\ i \end{pmatrix}$$

Table 6. Mass flows for lignin extraction process.

	$\dot{m}_i$ [g/batch]							
Material	**1a**	**2a**	**3a**	**4a**	**5a**	**6a**	**7a**	**8a**
Lignocellulosic biomass	138.95	-	-	-	-	-	-	-
H_2O	-	687.93	687.93		358.37	329.56		329.56
Na_2S	-	6.94	6.94	-	-	6.94	-	6.94
NaOH	-	23.61	23.61	-	-	23.61	-	23.61
Cellulose	-	-	58.36	58.36	-	-	-	-
H_2SO_4 15%	-	-	-	-	-	-	112.3	112.3
Hemicellulose	-	-	30.57	-	-	30.57	-	-
Sugars	-	-	-	-	-	-	-	30.57
H_2SO_4 5%		-	-	-	-	-	-	-
Lignin	-	-	33.35	--		33.35	-	33.35

$\dot{m}_i$ [g/batch]								
Material	**1a**	**2a**	**3a**	**4a**	**5a**	**6a**	**7a**	**8a**
Other substances from biomass	-	-	16.67	-	-	16.67	-	16.67
Total	138.95	718.48	857.43	58.36	358.37	440.7	112.3	553
Material	**9a**	**10a**	**11a**	**12a**	**13a**	**14a**	**1**	
Lignocellulosic biomass	-	-	-	-	-	-	-	
H_2O	329.56	-	-	-	-	-	-	
Na_2S	6.94	-	-	-	-	-	-	
NaOH	23.61	-	-	-	-	-	-	
Cellulose	-	-	-	-	-	-	-	
H_2SO_4 15%	112.3	-	-	-	-	-	-	
Hemicellulose	-	-	-	-	-	-	-	
Sugars	30.57	-	-	-	-	-	-	
H_2SO_4 5%	-	-	218.19	187	31.19	31.19	-	
Lignin	8.35	25	-	-	25	-	25	
Other substances from biomass	16.67	-	-	-	-	-	-	
Total	528	25	218.19	187	56.19	31.19	25	

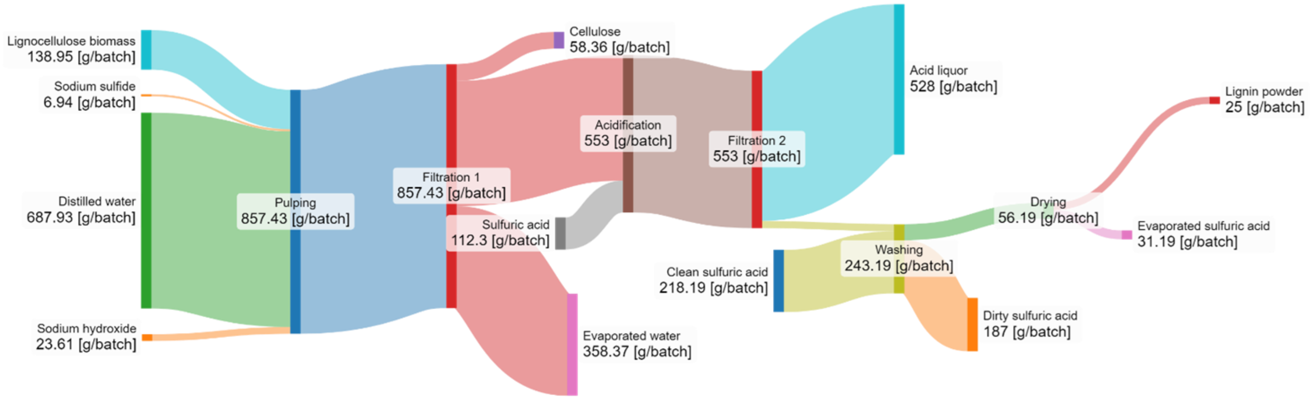

Figure 9. Sankey diagram for lignin extraction process.

Pulping

During this step, the lignocellulosic biomass that is introduced in the reactor is converted in cellulose, hemicellulose, lignin and other components. In this step there is no accumulation. Then:

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} + \begin{pmatrix} Rate\ of \\ generation\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix};\ \dot{m}_{1a} + \dot{m}_{2a} = \dot{m}_{3a}$$

$$\dot{m}_{1a,biomass} + \dot{m}_{2a,biomass} + \dot{m}_{generated\ biomass} = \dot{m}_{3a,biomass}$$

$$\dot{m}_{1a,biomass} = 138.95\ \left[\frac{g}{batch}\right]\ (E)$$

$$\dot{m}_{2a,biomass} = 0;\ \dot{m}_{3a,biomass} = 0$$

As all the lignocellulosic biomass is converted into other compounds, the following is assumed.

$$-\dot{m}_{1a,biomass} = \dot{m}_{generated\ biomass} = 138.95\ \left[\frac{g}{batch}\right]$$

To calculate the mass of the compounds derived from lignocellulosic biomass the following equations are followed.

$$\dot{m}_{1a,lignin} + \dot{m}_{2a,lignin} + \dot{m}_{generated\ lignin} = \dot{m}_{3a,lignin}$$

$$\dot{m}_{1a,cellulose} + \dot{m}_{2a,cellulose} + \dot{m}_{generated\ cellulose} = \dot{m}_{3a,cellulose}$$

$$\dot{m}_{1a,hemicellulose} + \dot{m}_{2a,hemicellulose} + \dot{m}_{generated\ hemicellulose} = \dot{m}_{3a,hemicellulose}$$

$$\dot{m}_{1a,other\ subs} + \dot{m}_{2a,other\ subs} + \dot{m}_{generated\ other\ subs} = \dot{m}_{3a,other\ subs}$$

In step 1a and step 2a, none of those components are introduced. Then:

$$\dot{m}_{1a,lignin} = \dot{m}_{2a,lignin} = 0$$

$$\dot{m}_{1a,cellulose} = \dot{m}_{2a,cellulose} = 0$$

$$\dot{m}_{1a,hemicellulose} = \dot{m}_{2a,hemicellulose} = 0$$

$$\dot{m}_{1a,other\ subs} = \dot{m}_{2a,other\ subs} = 0$$

The mass generated of the compounds derived from the separation of the lignocellulosic biomass can be calculated because the percentage of each compound is provided by the partners.

$$\dot{m}_{generated\ lignin} = \dot{m}_{1a,biomass} \cdot 0.24 = 33.35\ \left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{generated\ cellulose} = \dot{m}_{1a,biomass} \cdot 0.42 = 58.36\ \left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{generated\ hemicellulose} = \dot{m}_{1a,biomass} \cdot 0.22 = 30.57\ \left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{generated\ other\ subs} = \dot{m}_{1a,biomass} = 16.67\ \left[\frac{g}{batch}\right]\ (C)$$

Stream 3a for these compounds can be calculated:

$$\dot{m}_{3a,lignin} = 33.35\ \left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{3a,cellulose} = 58.36\ \left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{3a,hemicellulose} = 30.57\ \left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{3a,other\ subs} = 16.67\ \left[\frac{g}{batch}\right]\ (C)$$

The rest of the components introduced do not react, therefore the equations are expressed as follows.

$$\dot{m}_{1a,NaOH} + \dot{m}_{2a,NaOH} = \dot{m}_{3a,NaOH}$$

$$\dot{m}_{1a,H_2O} + \dot{m}_{2a,H_2O} = \dot{m}_{3a,H_2O}$$

$$\dot{m}_{1a,Na_2S} + \dot{m}_{2a,Na_2S} = \dot{m}_{3a,Na_2S}$$

$$\dot{m}_{2a,NaOH} = \dot{m}_{3a,NaOH} = 23.61 \left[\frac{g}{batch}\right] (E)$$

$$\dot{m}_{2a,H_2O} = \dot{m}_{3a,H_2O} = V_{2a,H_2O} \cdot \rho_{H_2O} = 0.690 \left[\frac{L}{batch}\right] \cdot 997 \left[\frac{g}{L}\right] = 687.93 \left[\frac{g}{batch}\right] (E)$$

$$\dot{m}_{2a,Na_2S} = \dot{m}_{3a,Na_2S} = 6.94 \left[\frac{g}{batch}\right] (E)$$

It is considered the density of water at 298 K, as it is the temperature in which the volume of water is measured [17].

Table 7. Mass flows for pulping step in lignin extraction process.

$\dot{m}_i$ [g/batch]			
Material	**1a (in)**	**2a (in)**	**3a (out)**
Lignocellulosic biomass	138.95	-	-
H_2O	-	687.93	687.93
Na_2S	-	6.94	6.94
NaOH	-	23.61	23.61
Cellulose	-	-	58.36
H_2SO_4 15%	-	-	-
Hemicellulose	-	-	30.57
Sugars	-	-	-
H_2SO_4 5%		-	-
Lignin	-	-	33.35
Other substances from biomass	-	-	16.67
Total	138.95	718.48	857.43

$$\dot{m}_{1a} + \dot{m}_{2a} = \dot{m}_{3a}; 138.95 + 718.48 = 857.43$$

Filtration 1

During this step there is no accumulation nor chemical reaction. Then:

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix}; \dot{m}_{3a} = \dot{m}_{4a} + \dot{m}_{5a} + \dot{m}_{6a}$$

Cellulose precipitates and is removed from the process. As in the previous step the system was heated, a portion of the water is evaporated.

$$\dot{m}_{3a,hemicellulose} = \dot{m}_{4a,hemicellulose} + \dot{m}_{5a,hemicellulose} + \dot{m}_{6a,hemicellulose}$$

$$\dot{m}_{3a,cellulose} = \dot{m}_{4a,cellulose} + \dot{m}_{5a,cellulose} + \dot{m}_{6a,cellulose}$$

$$\dot{m}_{3a,lignin} = \dot{m}_{4a,lignin} + \dot{m}_{5a,lignin} + \dot{m}_{6a,lignin}$$

$$\dot{m}_{3a,other\ subs} = \dot{m}_{4a,other\ subs} + \dot{m}_{5a,other\ subs} + \dot{m}_{6a,other\ subs}$$

$$\dot{m}_{3a,Na_2S} = \dot{m}_{4a,Na_2S} + \dot{m}_{5a,Na_2S} + \dot{m}_{6a,Na_2S}$$

$$\dot{m}_{3a,NaOH} = \dot{m}_{4a,NaOH} + \dot{m}_{5a,NaOH} + \dot{m}_{6a,NaOH}$$

$$\dot{m}_{3a,H_2O} = \dot{m}_{4a,H_2O} + \dot{m}_{5a,H_2O} + \dot{m}_{6a,H_2O}$$

All the cellulose is removed. Then:

$$\dot{m}_{6a,cellulose} = 0$$

$$\dot{m}_{3a,cellulose} = \dot{m}_{4a,cellulose} = 58.36 \left[\frac{g}{batch}\right] (C)$$

A portion the water is expelled from the system. A part of it is evaporated and the rest leaves the system by hydrating the cellulose. That quantity is calculated knowing that the mass of the acid liquor is 528 g, data provided by the partners. Therefore, the water that leaves the system is what follows.

$$\dot{m}_{5a,H_2O} = 358.37 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{3a,H_2O} - \dot{m}_{5a,H_2O} = \dot{m}_{6a,H_2O} = 687.93 - 358.37 = 329.56 \left[\frac{g}{batch}\right] (C)$$

The other components are not removed or introduced in the process. Therefore:

$$\dot{m}_{3a,hemicellulose} = \dot{m}_{6a,hemicellulose} = 30.57 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{3a,lignin} = \dot{m}_{6a,lignin} = 33.35 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{3a,other\ subs} = \dot{m}_{6a,other\ subs} = 16.67 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{3a,Na_2S} = \dot{m}_{6a,Na_2S} = 6.94 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{3a,NaOH} = \dot{m}_{6a,NaOH} = 23.61 \left[\frac{g}{batch}\right] (C)$$

Table 8. Mass flows for first filtration step in lignin extraction process.

	$\dot{m}_i$ [g/batch]			
Material	**3a (in)**	**4a (out)**	**5a (out)**	**6a (out)**
Lignocellulosic biomass	-	-	-	-
H_2O	687.93		358.37	329.56
Na_2S	6.94	-	-	6.94
NaOH	23.61	-	-	23.61
Cellulose	58.36	58.36	-	-
H_2SO_4 15%	-	-	-	-
Hemicellulose	30.57	-	-	30.57
Sugars	-	-	-	-
H_2SO_4 5%	-	-	-	-
Lignin	33.35	-		33.35
Other substances from biomass	16.67	-	-	16.67
Total	857.43	58.36	358.37	440.7

$$\dot{m}_{3a} = \dot{m}_{4a} + \dot{m}_{5a} + \dot{m}_{6a}; 857.43 = 58.36 + 358.37 + 440.7$$

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Acidification

During this step there is no accumulation. Sulfuric acid is added, which reacts with hemicellulose hydrolysing it to sugars.

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} + \begin{pmatrix} Rate\ of \\ generation\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix};\ \dot{m}_{6a} + \dot{m}_{7a} = \dot{m}_{8a}$$

$$\dot{m}_{6a,hemicellulose} + \dot{m}_{7a,hemicellulose} + \dot{m}_{generated\ hemicellulose} = \dot{m}_{8a,hemicellulose}$$

$$\dot{m}_{6a,lignin} + \dot{m}_{7a,lignin} = \dot{m}_{8a,lignin}$$

$$\dot{m}_{6a,other\ subs} + \dot{m}_{7a,other\ subs} = \dot{m}_{8a,other\ subs}$$

$$\dot{m}_{6a,Na_2S} + \dot{m}_{7a,Na_2S} = \dot{m}_{8a,Na_2S}$$

$$\dot{m}_{6a,NaOH} + \dot{m}_{7a,NaOH} = \dot{m}_{8a,NaOH}$$

$$\dot{m}_{6a,H_2O} + \dot{m}_{7a,H_2O} = \dot{m}_{8a,H_2O}$$

$$\dot{m}_{6a,sugar} + \dot{m}_{7a,sugar} + \dot{m}_{generated\ sugar} = \dot{m}_{8a,sugar}$$

$$\dot{m}_{6a,H_2SO_4,15\%} + \dot{m}_{7a,H_2SO_4,15\%} = \dot{m}_{8a,H_2SO_4,15\%}$$

Sulfuric acid hydrolyses hemicellulose and is recovered. Then:

$$\dot{m}_{7a,H_2SO_4,15\%} = \dot{m}_{8a,H_2SO_4,15\%} = V_{H_2SO_4,15\%} \cdot \rho_{H_2SO_4,15\%} = 0.1 \left[\frac{L}{batch}\right] \cdot 1123.45 \left[\frac{g}{L}\right] = 112.3 \left[\frac{g}{batch}\right]\ (E)$$

The density of pure sulfuric acid at 298 K, like water, is considered to be 1840 $\left[\frac{g}{L}\right]$ [18], so for 15% purity it will be:

$$\rho_{H_2SO_4,15\%} = 0.15 \cdot 1840 + 0.85 \cdot 997 = 1123.45 \left[\frac{g}{L}\right]$$

Hemicellulose is hydrolysed in the process. Then:

$$-\dot{m}_{6a,hemicellulose} = \dot{m}_{generated\ hemicellulose} = -30.57 \left[\frac{g}{batch}\right]\ (C)$$

The sign is negative because hemicellulose is not generated but hydrolysed.

Sugar generated is equal to the hemicellulose hydrolysed.

$$\dot{m}_{generated\ sugar} = \dot{m}_{8a,sugar} = 30.57 \left[\frac{g}{batch}\right]\ (C)$$

The rest of the components do not react, and they are not added or removed to the process.

$$\dot{m}_{6a,lignin} = \dot{m}_{8a,lignin} = 33.35 \left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{6a,other\ subs} = \dot{m}_{8a,other\ subs} = 16.67 \left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{6a,Na_2S} = \dot{m}_{8a,Na_2S} = 6.94 \left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{6a,NaOH} = \dot{m}_{8a,NaOH} = 23.61 \left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{6a,H_2O} = \dot{m}_{8a,H_2O} = 329.56 \left[\frac{g}{batch}\right]\ (C)$$

Table 9. Mass flows for acidification step in lignin extraction process.

$\dot{m}_i$ [g/batch]			
Material	**6a (in)**	**7a (in)**	**8a (out)**
Lignocellulosic biomass	-	-	-
H_2O	329.56		329.51
Na_2S	6.94	-	6.94
NaOH	23.61	-	23.61
Cellulose	-	-	-
H_2SO_4 15%	-	112.3	112.3
Hemicellulose	30.57	-	-
Sugars	-	-	30.57
H_2SO_4 5%	-	-	-
Lignin	33.35	-	33.35
Other substances from biomass	16.67	-	16.67
Total	440.7	112.3	553

$$\dot{m}_{6a} + \dot{m}_{7a} = \dot{m}_{8a};\ 440.7 + 112.3 = 553$$

Filtration 2

During this second filtration there are no chemical reaction nor accumulation. Acid liquor leaves the system, and the only compound that remains is lignin. The lignin that remains is the system is the same that is obtained at the end of the process, data that is provided by the partners.

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix};\ \dot{m}_{8a} = \dot{m}_{9a} + \dot{m}_{10a}$$

$$\dot{m}_{10a,lignin} = 25 \left[\frac{g}{batch}\right]\ (E)$$

$$\dot{m}_{8a,lignin} = \dot{m}_{9a,lignin} + \dot{m}_{10a,lignin}$$

$$\dot{m}_{9a,lignin} = \dot{m}_{8a,lignin} - \dot{m}_{10a,lignin} = 8.35 \left[\frac{g}{batch}\right]\ (C)$$

The rest of the compound leaves the process in the acid liquor.

$$\dot{m}_{8a,sugars} = \dot{m}_{9a,sugars} + \dot{m}_{10a,sugars}$$

$$\dot{m}_{8a,other\ subs} = \dot{m}_{9a,other\ subs} + \dot{m}_{10a,other\ subs}$$

$$\dot{m}_{8a,Na_2S} = \dot{m}_{9a,Na_2S} + \dot{m}_{10a,Na_2S}$$

$$\dot{m}_{8a,NaOH} = \dot{m}_{9a,NaOH} + \dot{m}_{10a,NaOH}$$

$$\dot{m}_{8a,H_2O} = \dot{m}_{9a,H_2O} + \dot{m}_{10a,H_2O}$$

$$\dot{m}_{8a,H_2SO_4,15\%} = \dot{m}_{9a,H_2SO_4,15\%} + \dot{m}_{10a,H_2SO_4,15\%}$$

$$\dot{m}_{8a,sugars} = \dot{m}_{9a,sugars} = 30.57 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{8a,other\ subs} = \dot{m}_{9a,other\ subs} = 16.67 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{8a,Na_2S} = \dot{m}_{9a,Na_2S} = 6.94 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{8a,NaOH} = \dot{m}_{9a,NaOH} = 23.61 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{8a,H_2O} = \dot{m}_{9a,H_2O} = 329.51 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{8a,H_2SO_4,15\%} = \dot{m}_{9a,H_2SO_4,15\%} = 112.3 \left[\frac{g}{batch}\right] (C)$$

The partners provided following data about the volume and the density of the acid liquor.

$$\dot{m}_{9a} = \dot{m}_{9a,sugars} + \dot{m}_{9a,other\ subs} + \dot{m}_{9a,Na_2S} + \dot{m}_{9a,NaOH} + \dot{m}_{9a,H_2O} + \dot{m}_{9a,H_2SO_4,15\%} + \dot{m}_{9a,lignin} = 528 \left[\frac{g}{batch}\right] (C)$$

$$V_{acid\ liquor} \cdot \rho_{acid\ liquor} = 0.48 \left[\frac{L}{batch}\right] \cdot 1100 \left[\frac{g}{L}\right] = 528 \left[\frac{g}{batch}\right] (E)$$

Total mass of stream 9 is the same as the mass of the acid liquor, proving that the water that leaves the system in the first filtration is well calculated.

Table 10. Mass flows for second filtration step in lignin extraction process.

$\dot{m}_i$ [g/batch]			
Material	**8a (in)**	**9a (out)**	**10a (out)**
Lignocellulosic biomass	-	-	-
H_2O	329.56	329.56	-
Na_2S	6.94	6.94	-
NaOH	23.61	23.61	-
Cellulose	-	-	-
H_2SO_4 15%	112.3	112.3	-
Hemicellulose	-	-	-
Sugars	30.57	30.57	-
H_2SO_4 5%	-	-	-
Lignin	33.35	8.35	25
Other substances from biomass	16.67	16.67	
Total	553	528	25

$$\dot{m}_{8a} = \dot{m}_{9a} + \dot{m}_{10a};\ 553 = 528 + 25$$

Washing

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix};\ \dot{m}_{10a} + \dot{m}_{11a} = \dot{m}_{12a} + \dot{m}_{13a}$$

The product is washed with H_2SO_4 at 5%. The stream corresponding to the clean liquid (11a) is calculated using density from bibliography for H_2SO_4 at 5%. The density of the dirty stream (12a) is obtained experimentally.

Using the same reference used for acidification, we can estimate the value of sulfuric acid at 5%:

$$\rho_{H_2SO_4,5\%} = 0.05 \cdot 1840 + 0.95 \cdot 997 = 1039.15 \left[\frac{g}{L}\right]$$

$$\dot{m}_{11a,H_2SO_4,5\%} = 0.21 \left[\frac{L}{batch}\right] \cdot 1039 \left[\frac{g}{L}\right] = 218.19 \left[\frac{g}{batch}\right] \ (E)$$

$$\dot{m}_{12a,H_2SO_4,5\%} = 0.17 \left[\frac{L}{batch}\right] \cdot 1100 \left[\frac{g}{L}\right] = 187.0 \left[\frac{g}{batch}\right] \ (E)$$

Therefore, for sulfuric acid, the equation obtained is the following.

$$\dot{m}_{10a,H_2SO_4,5\%} + \dot{m}_{11a,H_2SO_4,5\%} = \dot{m}_{12a,H_2SO_4,5\%} + \dot{m}_{13a,H_2SO_4,5\%}$$

$$\dot{m}_{13a,H_2SO_4,5\%} = \dot{m}_{11a,H_2SO_4,5\%} - \dot{m}_{12a,H_2SO_4,5\%} = 31.19 \left[\frac{g}{batch}\right] \ (C)$$

Lignin is the same as in the previous step.

$$\dot{m}_{10a,lignin} + \dot{m}_{11a,lignin} = \dot{m}_{12a,lignin} + \dot{m}_{13a,lignin}$$

$$\dot{m}_{10a,lignin} = \dot{m}_{13a,lignin} = 25 \left[\frac{g}{batch}\right] \ (C)$$

Table 11. Mass flows for washing step in lignin extraction process.

	$\dot{m}_i$ [g/batch]			
Material	**10a (in)**	**11a (in)**	**12a (out)**	**13a (out)**
Lignocellulosic biomass	-	-	-	-
H_2O	-	-	-	-
Na_2S	-	-	-	-
NaOH	-	-	-	-
Cellulose	-	-	-	-
H_2SO_4 15%	-	-	-	-
Hemicellulose	-	-	-	-
Sugars	-	-	-	-
H_2SO_4 5%	-	218.19	187	31.19
Lignin	25	-	-	25
Other substances from biomass	-	-	-	-
Total	25	218.19	187	56.19

$$\dot{m}_{10a} + \dot{m}_{11a} = \dot{m}_{12a} + \dot{m}_{13a}; 25 + 218.19 = 187 + 56.19$$

Drying

In this step, sulfuric acid is evaporated, and the final lignin powder is obtained.

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix}; \ \dot{m}_{13a} = \dot{m}_{14a} + \dot{m}_1$$

$$\dot{m}_{1,lignin} = 25\left[\frac{g}{batch}\right]\ (E)$$

$$\dot{m}_{13a,lignin} = 25\left[\frac{g}{batch}\right]\ (C)$$

Lignin mass that enters the drying step matches the mass data that the partners provide. Therefore, calculations should be correct.

Sulfuric acid is evaporated during this step. At the end of the process there is not any rest, meaning that:

$$\dot{m}_{13a,H_2SO_4,5\%} = \dot{m}_{14a,H_2SO_4,5\%} = 31.19\left[\frac{g}{batch}\right]\ (C)$$

Table 12. Mass flows for drying step lignin extraction process.

$\dot{m}_i$ [g/batch]			
Material	**13a (in)**	**14a (out)**	**1 (out)**
Lignocellulosic biomass	-	-	-
H_2O	-	-	-
Na_2S	-	-	-
NaOH	-	-	-
Cellulose	-	-	-
H_2SO_4 15%	-	-	-
Hemicellulose	-	-	-
Sugars	-	-	-
H_2SO_4 5%	31.19	31.19	-
Lignin	25	-	25
Other substances from biomass	-	-	-
Total	56.19	31.19	25

$$\dot{m}_{13a} = \dot{m}_{14a} + \dot{m}_1;\ 56.19 = 31.19 + 25$$

Rubber functionalisation

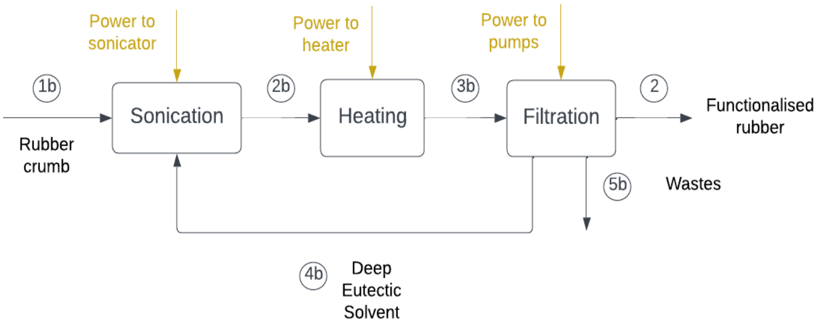

Figure 10. PFD for rubber functionalisation process.

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$$\begin{pmatrix}Rate\ of\\ input\ of\ i\end{pmatrix}-\begin{pmatrix}Rate\ of\\ output\ of\ i\end{pmatrix}+\begin{pmatrix}Rate\ of\\ generation\ of\ i\end{pmatrix}=\begin{pmatrix}Rate\ of\\ accumulation\ of\ i\end{pmatrix}$$

During the rubber functionalisation process there are no chemical reactions nor accumulations. Hence:

$$\begin{pmatrix}Rate\ of\\ input\ of\ i\end{pmatrix}=\begin{pmatrix}Rate\ of\\ output\ of\ i\end{pmatrix}$$

Table 13. Mass flows for rubber functionalisation process.

	$\dot{m}_i$ [g/batch]					
Material	**1b**	**2b**	**3b**	**4b**	**5b**	**2**
Rubber crumb	100	100	100	-	20	80
DES	-	2000	2000	2000	-	-
Total	100	2100	2100	2000	20	80

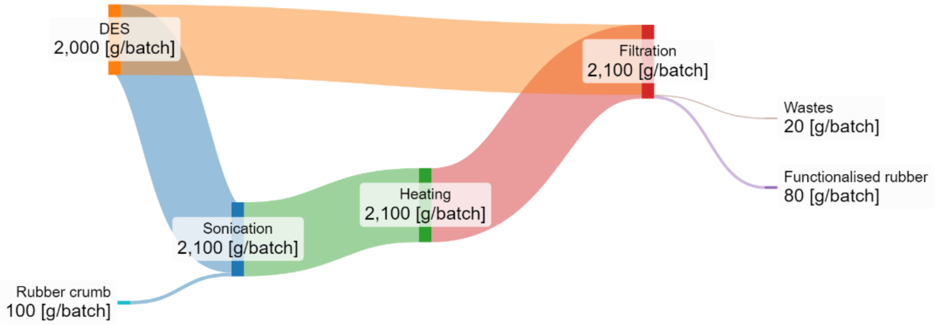

Figure 11. Sankey diagram for rubber functionalisation.

Sonication

In this step, rubber crumb is sonicated. DES is recovered from stream 4b. The first time the process takes place, new DES is used. Data about the mass of those compounds is provided by the partners.

$$\begin{pmatrix}Rate\ of\\ input\ of\ i\end{pmatrix}=\begin{pmatrix}Rate\ of\\ output\ of\ i\end{pmatrix};\ \dot{m}_{1b}+\dot{m}_{4b}=\dot{m}_{2b}$$

$$\dot{m}_{1b,DES}+\dot{m}_{4b,DES}=\dot{m}_{2b,DES}$$

$$\dot{m}_{1b,rubber}+\dot{m}_{4b,rubber}=\dot{m}_{2b,rubber}$$

$$\dot{m}_{1b,rubber}=\dot{m}_{2b,rubber}=100.0\left[\frac{g}{batch}\right]\ (E)$$

$$\dot{m}_{4b,DES}=\dot{m}_{2b,DES}=2000.0\left[\frac{g}{batch}\right]\ (E)$$

Table 14. Mass flows for sonication step in rubber functionalisation process.

$\dot{m}_i$ [g/batch]			
Material	**1b (in)**	**2b (out)**	**4b (in)**
Rubber crumb	100	100	-
DES	-	2000	2000
Total	100	2100	2000

$$\dot{m}_{1b} + \dot{m}_{4b} = \dot{m}_{2b};\, 100 + 2000 = 2100$$

Heating

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix};\ \dot{m}_{2b} = \dot{m}_{3b}$$

During the heating process there are not any changes in the composition.

$$\dot{m}_{2b,rubber} = \dot{m}_{3b,rubber} = 100.0\ \left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{2b,DES} = \dot{m}_{3b,DES} = 2000.0\ \left[\frac{g}{batch}\right]\ (C)$$

During heating step, gases are produced, but they are not significant enough to be considered.

Table 15. Mass flows for heating step in rubber functionalisation process.

$\dot{m}_i$ [g/batch]		
Material	**2b (in)**	**3b (out)**
Rubber crumb	100	100
DES	2000	2000
Total	2100	2100

$$\dot{m}_{2b} = \dot{m}_{3b};\, 2100 = 2100$$

Filtration

In this step, devulcanized rubber crumb is produced. Wastes of the rubber crumb are generated. There are not chemical reactions nor accumulation. Data about the final devulcanized rubber obtained and the wastes is provided by the partners.

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix};\ \dot{m}_{3b} = \dot{m}_{4b} + \dot{m}_{5b} + \dot{m}_{2}$$

$$\dot{m}_{5b,rubber} = 20\left[\frac{g}{batch}\right]\ (E)$$

$$\dot{m}_{2,rubber} = 80\left[\frac{g}{batch}\right]\ (E)$$

$$\dot{m}_{3b,rubber} = \dot{m}_{5b,rubber} + \dot{m}_{2,rubber} = 100.0\ \left[\frac{g}{batch}\right]\ (C)$$

DES is recovered and use again in the first step of this process

$$\dot{m}_{3b,DES} = \dot{m}_{4b,DES} = 2000.0 \left[\frac{g}{batch}\right] (E)$$

Table 16. Mass flows for filtration step in rubber functionalisation process.

$\dot{m}_i$ [g/batch]				
Material	**3b (in)**	**4b (out)**	**5b (out)**	**2 (out)**
Rubber crumb	100	-	20	80
DES	2000	2000	-	-
Total	2100	2000	20	80

$$\dot{m}_{3b} = \dot{m}_{4b} + \dot{m}_{5b} + \dot{m}_2; 2100 = 2000 + 20 + 80$$

Rubber panel production

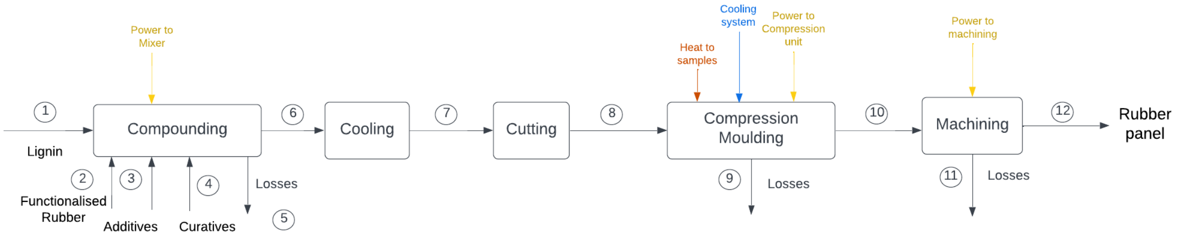

Figure 12. PFD for rubber panel production process.

There are not chemical reactions nor accumulations.

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} - \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix} + \begin{pmatrix} Rate\ of \\ generation\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ accumulation\ of\ i \end{pmatrix}$$

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix}$$

Table 17. Mass flows for rubber panel production process.

$\dot{m}_i$ [g/batch]						
Material	**1**	**2**	**3**	**4**	**5**	**6**
Lignin	25	-	-	-	1.25	23.75
Devulcanized rubber crumb	-	80	-	-	4.00	76.00
Natural rubber crumb	-	20	-	-	1.00	19.00
Low lead zinc oxide	-	-	5	-	0.25	4.75
Stearic acid	-	-	1	-	0.05	0.95
MBTS-75	-	-	-	0.5	0.03	0.48
Mesh sulphur	-	-	-	2.5	0.13	2.38
Total	25	100	6	3	6.7	127.3

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	$\dot{m}_i$ [g/batch]					
Material	**7**	**8**	**9**	**10**	**11**	**12**
Lignin	23.75	23.75	1.19	22.56	1.13	21.43
Devulcanized rubber crumb	76.00	76.00	3.8	72.2	3.61	68.59
Natural rubber crumb	19.00	19.00	0.95	18.05	0.9	17.15
Low lead zinc oxide	4.75	4.75	0.24	4.51	0.23	4.29
Stearic acid	0.95	0.95	0.05	0.9	0.05	0.86
MBTS-75	0.48	0.48	0.02	0.45	0.02	0.43
Mesh sulphur	2.38	2.38	0.12	2.26	0.11	2.14
Total	127.3	127.3	6.37	120.93	6.05	114.89

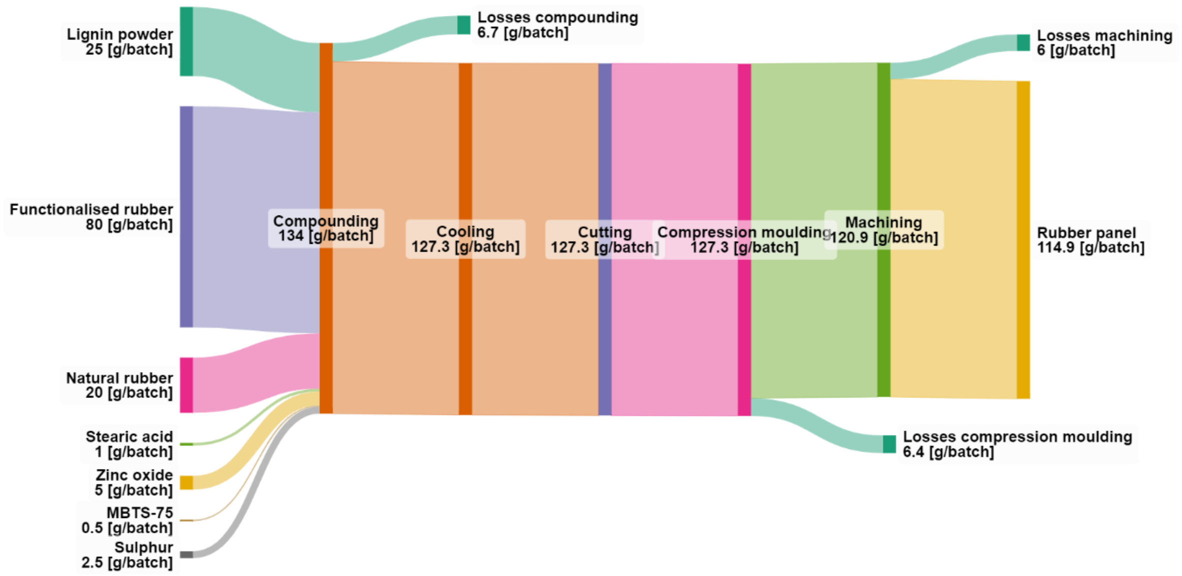

Figure 13. Sankey diagram for rubber panel production.

Compounding

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix};\ \dot{m}_1 + \dot{m}_2 + \dot{m}_3 + \dot{m}_4 = \dot{m}_5 + \dot{m}_6$$

In this step, all the compounds involved in the process are introduced in the mixer. Data about the quantity used is provided by the partners.

$$\dot{m}_{1,lignin} + \dot{m}_{2,lignin} + \dot{m}_{3,lignin} + \dot{m}_{4,lignin} = \dot{m}_{5,lignin} + \dot{m}_{6,lignin}$$

$$\dot{m}_{1,devul\ rubber} + \dot{m}_{2,devul\ rubber} + \dot{m}_{3,devul\ rubber} + \dot{m}_{4,devul\ rubber} = \dot{m}_{5,devul\ rubber} + \dot{m}_{6,devul\ rubber}$$

$$\dot{m}_{1,nat\ rubber} + \dot{m}_{2,nat\ rubber} + \dot{m}_{3,nat\ rubber} + \dot{m}_{4,nat\ rubber} = \dot{m}_{5,nat\ rubber} + \dot{m}_{6,nat\ rubber}$$

$$\dot{m}_{1,zinc\ oxide} + \dot{m}_{2,zinc\ oxide} + \dot{m}_{3,zinc\ oxide} + \dot{m}_{4,zinc\ oxide} = \dot{m}_{5,zinc\ oxide} + \dot{m}_{6,zinc\ oxide}$$

$$\dot{m}_{1,stearic\ acid} + \dot{m}_{2,stearic\ acid} + \dot{m}_{3,stearic\ acid} + \dot{m}_{4,stearic\ acid} = \dot{m}_{5,stearic\ acid} + \dot{m}_{6,stearic\ acid}$$

$$\dot{m}_{1,MBTS-75} + \dot{m}_{2,MBTS-75} + \dot{m}_{3,MBTS-75} + \dot{m}_{4,MBTS-75} = \dot{m}_{5,MBTS-75} + \dot{m}_{6,MBTS-75}$$

$$\dot{m}_{1,sulphur} + \dot{m}_{2,sulphur} + \dot{m}_{3,sulphur} + \dot{m}_{4,sulphur} = \dot{m}_{5,sulphur} + \dot{m}_{6,sulphur}$$

Losses are expected to be around 5% of the total mass. It is assumed that all the compounds are lost at the same percentage.

$$\dot{m}_{1,lignin} = 25\left[\frac{g}{batch}\right]\ (E)$$

$$\dot{m}_{2,devul\ rubber} = 80\left[\frac{g}{batch}\right]\ (E)$$

$$\dot{m}_{2,nat\ rubber} = 20\left[\frac{g}{batch}\right]\ (E)$$

$$\dot{m}_{3,zinc\ oxide} = 5\left[\frac{g}{batch}\right]\ (E)$$

$$\dot{m}_{3,stearic\ acid} = 1\left[\frac{g}{batch}\right] (E)$$

$$\dot{m}_{4,MBTS-75} = 0.5\left[\frac{g}{batch}\right] (E)$$

$$\dot{m}_{4,sulphur} = 2.5\left[\frac{g}{batch}\right] (E)$$

$$\dot{m}_{5,lignin} = \dot{m}_{1,lignin} \cdot 0.05 = 1.25\left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{5,devul\ rubber} = \dot{m}_{2,devul\ rubber} \cdot 0.05 = 4\left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{5,nat\ rubber} = \dot{m}_{2,nat\ rubber} \cdot 0.05 = 1\left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{5,zinc\ oxide} = \dot{m}_{3,zinc\ oxide} \cdot 0.05 = 0.25\left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{5,stearic\ acid} = \dot{m}_{3,stearic\ acid} \cdot 0.05 = 0.05\left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{5,MBTS-75} = \dot{m}_{4,MBTS-75} \cdot 0.05 = 0.03\left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{5,sulphur} = \dot{m}_{4,sulphur} \cdot 0.05 = 0.13\left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{1,lignin} - \dot{m}_{5,lignin} = \dot{m}_{6,lignin} = 23.75\left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{2,devul\ rubber} - \dot{m}_{5,devul\ rubber} = \dot{m}_{6,devul\ rubber} = 76\left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{2,nat\ rubber} - \dot{m}_{5,nat\ rubber} = \dot{m}_{6,nat\ rubber} = 19\left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{3,zinc\ oxide} - \dot{m}_{5,zinc\ oxide} = \dot{m}_{6,zinc\ oxide} = 4.75\left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{3,stearic\ acid} - \dot{m}_{5,stearic\ acid} = \dot{m}_{6,stearic\ acid} = 0.95\left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{4,MBTS-75} - \dot{m}_{5,MBTS-75} = \dot{m}_{6,MBTS-75} = 0.48\left[\frac{g}{batch}\right](C)$$

$$\dot{m}_{4,sulphur} - \dot{m}_{5,sulphur} = \dot{m}_{6,sulphur} = 2.38\left[\frac{g}{batch}\right](C)$$

During compounding, losses are estimated at a 5% of the total compound. Enough to be considered in the calculation.

Table 18. Mass flows for compounding step in rubber panel production process.

$\dot{m}_i$ [g/batch]						
Material	**1**	**2**	**3**	**4**	**5**	**6**
Lignin	25	-	-	-	1.25	23.75
Devulcanized rubber crumb	-	80	-	-	4.00	76.00
Natural rubber crumb	-	20	-	-	1.00	19.00
Low lead zinc oxide	-	-	5	-	0.25	4.75
Stearic acid	-	-	1	-	0.05	0.95
MBTS-75	-	-	-	0.5	0.03	0.48
Mesh sulphur	-	-	-	2.5	0.13	2.38
Total	25	100	6	3	6.7	127.3

$$\dot{m}_1 + \dot{m}_2 + \dot{m}_3 + \dot{m}_4 = \dot{m}_5 + \dot{m}_6;\, 25 + 100 + 6 + 3 = 6.8 + 127.3$$

Cooling

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix};\ \dot{m}_6 = \dot{m}_7$$

This step takes place at ambient temperature. There are no losses.

$$\dot{m}_{7,lignin} = \dot{m}_{6,lignin} = 23.75\left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{7,devul\ rubber} = \dot{m}_{6,devul\ rubber} = 76\left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{7,nat\ rubber} = \dot{m}_{6,nat\ rubber} = 19\left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{7,zinc\ oxide} = \dot{m}_{6,zinc\ oxide} = 4.75\left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{7,stearic\ acid} = \dot{m}_{6,stearic\ acid} = 0.95\left[\frac{g}{batch}\right](C)$$

$$\dot{m}_{7,MBTS-75} = \dot{m}_{6,MBTS-75} = 0.48\left[\frac{g}{batch}\right](C)$$

$$\dot{m}_{7,sulphur} = \dot{m}_{6,sulphur} = 2.38\left[\frac{g}{batch}\right](C)$$

Table 19. Mass flows for cooling step in rubber panel production process.

$\dot{m}_i$ [g/batch]		
Material	**6**	**7**
Lignin	23.75	23.75
Devulcanized rubber crumb	76.00	76.00
Natural rubber crumb	19.00	19.00
Low lead zinc oxide	4.75	4.75
Stearic acid	0.95	0.95
MBTS-75	0.48	0.48
Mesh sulphur	2.38	2.38
Total	127.3	127.3

$$\dot{m}_6 = \dot{m}_7;\ 127.3 = 127.3$$

Cutting

During the cutting, there are not significant losses. Also, there are not chemical reactions nor accumulations.

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix};\ \dot{m}_7 = \dot{m}_8$$

$$\dot{m}_{7,lignin} = \dot{m}_{8,lignin} = 23.75\left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{7,devul\ rubber} = \dot{m}_{8,devul\ rubber} = 76\left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{7,nat\ rubber} = \dot{m}_{8,nat\ rubber} = 19\left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{7,zinc\ oxide} = \dot{m}_{8,zinc\ oxide} = 4.75\left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{7,stearic\ acid} = \dot{m}_{8,stearic\ acid} = 0.95\left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{7,MBTS-75} = \dot{m}_{8,MBTS-75} = 0.48\left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{7,sulphur} = \dot{m}_{8,sulphur} = 2.38\left[\frac{g}{batch}\right] (C)$$

Table 20. Mass flows for cutting step in rubber panel production process.

$\dot{m}_i$ [g/batch]		
Material	**7**	**8**
Lignin	23.75	23.75
Devulcanized rubber crumb	76.00	76.00
Natural rubber crumb	19.00	19.00

$\dot{m}_i$ [g/batch]		
Material	**7**	**8**
Low lead zinc oxide	4.75	4.75
Stearic acid	0.95	0.95
MBTS-75	0.48	0.48
Mesh sulphur	2.38	2.38
Total	127.3	127.3

$$\dot{m}_7 = \dot{m}_8;\ 127.3 = 127.3$$

Compression moulding

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix};\ \dot{m}_8 = \dot{m}_9 + \dot{m}_{10}$$

During compression moulding, losses are estimated at a 5% of the inlet stream. Gases are evaporated during this step, but the emissions were not significant enough to be considered.

$$\dot{m}_{9,lignin} = \dot{m}_{8,lignin} \cdot 0.05 = 1.19 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{9,devul\ rubber} = \dot{m}_{8,devul\ rubber} \cdot 0.05 = 3.8 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{9,nat\ rubber} = \dot{m}_{8,nat\ rubber} \cdot 0.05 = 0.95 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{9,zinc\ oxide} = \dot{m}_{8,zinc\ oxide} \cdot 0.05 = 0.24 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{9,stearic\ acid} = \dot{m}_{8,stearic\ acid} \cdot 0.05 = 0.05 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{9,MBTS-75} = \dot{m}_{8,MBTS-75} \cdot 0.05 = 0.02 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{9,sulphur} = \dot{m}_{8,sulphur} \cdot 0.05 = 0.11 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{8,lignin} - \dot{m}_{9,lignin} = \dot{m}_{10,lignin} = 22.56 \left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{8,devul\ rubber} - \dot{m}_{9,devul\ rubber} = \dot{m}_{10,devul\ rubber} = 72.2 \left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{8,nat\ rubber} - \dot{m}_{9,nat\ rubber} = \dot{m}_{10,nat\ rubber} = 18.05 \left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{8,zinc\ oxide} - \dot{m}_{9,zinc\ oxide} = \dot{m}_{10,zinc\ oxide} = 4.51 \left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{8,stearic\ acid} - \dot{m}_{9,stearic\ acid} = \dot{m}_{10,stearic\ acid} = 0.9 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{8,MBTS-75} - \dot{m}_{9,MBTS-75} = \dot{m}_{10,MBTS-75} = 0.45 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{8,sulphur} - \dot{m}_{9,sulphur} = \dot{m}_{10,sulphur} = 2.26 \left[\frac{g}{batch}\right] (C)$$

Table 21. Mass flows for compression moulding step in rubber panel production process.

$\dot{m}_i$ [g/batch]			
Material	**8**	**9**	**10**
Lignin	23.75	1.19	22.56
Devulcanized rubber crumb	76.00	3.8	72.2
Natural rubber crumb	19.00	0.95	18.05
Low lead zinc oxide	4.75	0.24	4.51
Stearic acid	0.95	0.05	0.9
MBTS-75	0.48	0.02	0.45
Mesh sulphur	2.38	0.12	2.26
Total	127.3	6.4	120.9

$$\dot{m}_8 = \dot{m}_9 + \dot{m}_{10}; 127.3 = 6.4 + 120.9$$

Machining

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix}; \dot{m}_{10} = \dot{m}_{11} + \dot{m}_{12}$$

During machining, losses are estimated at a 5% of the inlet stream.

$$\dot{m}_{11,lignin} = \dot{m}_{10,lignin} \cdot 0.05 = 1.13 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{11,devul\ rubber} = \dot{m}_{10,devul\ rubber} \cdot 0.05 = 3.61 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{11,nat\ rubber} = \dot{m}_{10,nat\ rubber} \cdot 0.05 = 0.9 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{11,zinc\ oxide} = \dot{m}_{10,zinc\ oxide} \cdot 0.05 = 0.23 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{11,stearic\ acid} = \dot{m}_{10,stearic\ acid} \cdot 0.05 = 0.05 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{11,MBTS-75} = \dot{m}_{10,MBTS-75} \cdot 0.05 = 0.02 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{11,sulphur} = \dot{m}_{10,sulphur} \cdot 0.05 = 0.11 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{10,lignin} - \dot{m}_{11,lignin} = \dot{m}_{12,lignin} = 21.43 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{10,devul\ rubber} - \dot{m}_{11,devul\ rubber} = \dot{m}_{12,devul\ rubber} = 68.59 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{10,nat\ rubber} - \dot{m}_{11,nat\ rubber} = \dot{m}_{12,nat\ rubber} = 17.15 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{10,zinc\ oxide} - \dot{m}_{11,zinc\ oxide} = \dot{m}_{12,zinc\ oxide} = 4.29\left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{10,stearic\ acid} - \dot{m}_{11,stearic\ acid} = \dot{m}_{12,stearic\ acid} = 0.86\left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{10,MBTS-75} - \dot{m}_{11,MBTS-75} = \dot{m}_{12,MBTS-75} = 0.43\left[\frac{g}{batch}\right]\ (C)$$

$$\dot{m}_{10,sulphur} - \dot{m}_{11,sulphur} = \dot{m}_{12,sulphur} = 2.14\left[\frac{g}{batch}\right]\ (C)$$

Table 22. Mass flows for machining step in rubber panel production process.

$\dot{m}_i$ [g/batch]			
Material	**10**	**11**	**12**
Lignin	22.56	1.13	21.43
Devulcanized rubber crumb	72.2	3.61	68.59
Natural rubber crumb	18.05	0.9	17.15
Low lead zinc oxide	4.51	0.23	4.29
Stearic acid	0.9	0.05	0.86
MBTS-75	0.45	0.02	0.43
Mesh sulphur	2.26	0.11	2.14
Total	120.9	6	114.9

$$\dot{m}_{10} = \dot{m}_{11} + \dot{m}_{12};\ 120.9 = 6 + 114.9$$

Energy balance

The equation for the energy balance is described in the methodology. It is assumed that the kinetic and potential energy are negligible for all the processes described in WP3.

$$\sum_k (\dot{m}_k \cdot h_k)_{in} - \sum_k (\dot{m}_k \cdot h_k)_{out} + \dot{Q}_{int} - P_{sys}\frac{dV_{sys}}{dt} + \dot{W}_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = \frac{d(m \cdot u)_{sys}}{dt}$$

Even though the process is not steady state, it is considered that there is no accumulation, meaning that:

$$\frac{d(m \cdot u)_{sys}}{dt} = 0$$

Also, there are not changes in volume, which implies the following.

$$P_{sys}\frac{dV_{sys}}{dt} = 0$$

For all the processes that comprise WP3, the equation used is the one that follows.

$$\sum_k (\dot{m}_k \cdot h_k)_{in} - \sum_k (\dot{m}_k \cdot h_k)_{out} + \dot{Q}_{int} + \dot{W}_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

Lignin extraction

Pulping

In pulping step, all the compounds are introduced at room temperature, and inside the reactor, they are heated to 448 K, which is the temperature of the outlet stream. Data about the power of the reactor is provided by the partners. The reactor also acts as a heater of the samples.

The temperature of the compounds that enter the system room temperature (298 K), which is the same as the reference temperature. Therefore:

$$\sum_k (m_k \cdot h_k)_{in} = 0$$

$$\begin{aligned}\sum_k (m_k \cdot h_k)_{out} = \Big[& \left(m_{lignin}\right)_{3a} \cdot C_{P,lignin,3a} + (m_{cellulose})_{3a} \cdot C_{P,cellulose,3a} + (m_{hemicellulose})_{3a} \cdot C_{P,hemicellulose,3a} \\ & + (m_{other\ subs})_{3a} \cdot C_{P,other\ subs,3a} + (m_{NaOH})_{3a} \cdot C_{P,NaOH,3a} + \left(m_{Na_2S}\right)_{3a} \cdot C_{P,Na_2S,3a} + \left(m_{H_2O}\right)_{3a} \cdot C_{P,H_2O,3a}\Big] \\ & \cdot (T_{3a} - T_{ref}) \\ & = [1.54 \cdot 33.35 + 1.21 \cdot 58.36 + 1.31 \cdot 30.57 + 0.95 \cdot 16.65 + 1.75 \cdot 23.61 + 1.18 \cdot 6.94 + 4.46 \cdot 687.93] \\ & \cdot (448 - 298) = \ 493.85\ kJ\end{aligned}$$

Specific heats for the components were found in bibliography. For lignin, cellulose, hemicellulose and other substances, example values were chosen.

$C_{P,lignin} = 1.54\ \frac{J}{g \cdot K}$ [19]

$C_{P,hemicellulose} = 1.31\ \frac{J}{g \cdot K}$ [19]

$C_{P,cellulose} = 1.21\ \frac{J}{g \cdot K}$ [19]

$C_{P,other\ subs} = 0.95\ \frac{J}{g \cdot K}$ [20]

For other substances, the specific heat value corresponds to ashes, which is the main component.

$C_{P,NaOH} = 1.75\ \frac{J}{g \cdot K}$ [21]

$C_{P,Na_2S} = \ 1.18 \frac{J}{g \cdot K}$ [21]

$C_{P,H_2O} = 4.46\ \frac{J}{g \cdot K}$ [21]

The reactor generates mechanical power and heat in the system. There is no data on what percentage of the power required by the reactor is for heating or mixing. Therefore, it will be considered that all the power is for mixing the components. An efficiency of 85% is considered, as explained in section 2.2.1.

$$W_{shaft} = \eta_{reactor} \cdot W_{reactor} = 0.85 \cdot 3.68\ [kW] \cdot 3\ [h] \cdot \frac{3600}{1} \left[\frac{kJ}{kWh}\right] = 33782\ kJ$$

It is important to note that during this process, some reactions occur. The term related is impossible to calculate, since there is not sufficient data in bibliography. The enthalpy of the reaction should be measured experimentally to obtain an accurate approximation. Therefore, for the purpose of the calculations, it is going to be assumed that the term is equal to zero, in order to calculate the heat exchange.

$$Q_{int} = -W_{shaft} + \sum_k (\dot{m}_k \cdot h_k)_{out} = -33288\ \mathrm{kJ}$$

Table 23. Energy contributions for the pulping step in lignin extraction process.

Energy contributions	Pulping
$(m_k \cdot h_k)_{in}$ [kJ]	0
$(m_k \cdot h_k)_{out}$ [kJ]	493.85
Q_{int} [kJ]	-33288
W_{shaft} [kJ]	33782
$\sum \Delta H_R^{Tref}$ [kJ]	Unknown

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0;\ -494 - 33288 + 33782 = 0$$

Filtration 1

In the first filtration step, the energy derived from the mass flow for the inlet stream has the same value as the outlet stream in the previous step, as the components and temperatures are the same. Filtration is done by a Büchner funnel. It is assumed that the filtration requires 2 W [22], and the process takes place in 30 minutes.

$$\sum_k (m_k \cdot h_k)_{in,filtration\ 1} = \sum_k (m_k \cdot h_k)_{out,pulping} = 493.85\ kJ$$

Cellulose and the remaining liquid are removed when reached room temperature, meaning that the only compound that leaves the system at a temperature difference to the reference one is water:

$$\sum_k (m_k \cdot h_k)_{out} = \left[\left(m_{H_2O}\right)_3 \cdot C_{P,H_2O,3}\right] \cdot \left(T_5 - T_{ref}\right) = [4.46 \cdot 358.37] \cdot (448 - 298) = 239.75\ kJ$$

The filter generates mechanical power in the system. An efficiency of 85% is considered, as explained in section 2.2.1.

$$W_{shaft} = \eta_{filter} \cdot W_{filter} = 0.85 \cdot 0.002\ [kW] \cdot 0.5\ [h] \cdot \frac{3600}{1} \left[\frac{kJ}{kWh}\right] = 3.06\ kJ$$

There are no chemical reactions during the process:

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

$$Q_{int} = -\mathrm{W}_{shaft} - \sum_k (m_k \cdot h_k)_{in} + \sum_k (\mathrm{m}_k \cdot h_k)_{out} = -257.16\ kJ$$

Table 24. Energy contributions for the first filtration step in lignin extraction process.

Energy contributions	Filtration 1
$(m_k \cdot h_k)_{in}$ [kJ]	493.85
$(m_k \cdot h_k)_{out}$ [kJ]	239.75

Energy contributions	Filtration 1
Q_{int} [kJ]	-257.16
W_{shaft} [kJ]	3.06
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0;\ 493.85 - 239.75 - 257.16 + 3.06 = 0$$

Acidification

The entire step takes place at ambient temperature, meaning that:

$$\sum_k (m \cdot h_k)_{in} = \sum_k (m_k \cdot h_k)_{out} = 0$$

Acidification is done with a magnetic stirrer. They have a consumption of 2 W [23], and the process is assumed to take place in 30 minutes. An efficiency of 85% is considered, as explained in section 2.2.1.

$$W_{shaft} = \eta_{mixer} \cdot W_{mixer} = 0.85 \cdot 0.002\ [kW] \cdot 0.5\ [h] \cdot \frac{3600}{1} \left[\frac{kJ}{kWh}\right] = 3.06\ kJ$$

There are no chemical reactions, meaning that:

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

Therefore:

$$Q_{int} = -\mathrm{W}_{shaft} = 3.06\ kJ$$

Table 25. Energy contributions for the acidification step in lignin extraction process.

Energy contributions	Acidification
$(m_k \cdot h_k)_{in}$ [kJ]	0
$(m_k \cdot h_k)_{out}$ [kJ]	0
Q_{int} [kJ]	-3.06
W_{shaft} [kJ]	3.06
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + \mathrm{Q}_{int} + \mathrm{W}_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0;\ -3.06 + 3.06 = 0$$

Filtration 2

The second filtration takes place at room temperature, meaning that all the inlet and outlet streams are at 298 K, reference temperature.

$$\sum_k (m_k \cdot h_k)_{in} = \sum_k (m_k \cdot h_k)_{out} = 0$$

Filtration is done by a Büchner funnel. It is assumed that the filtration requires 2 W [22], and the process takes place in 30 minutes. The mechanical power generated in the system is assumed to have an efficiency of 85%, as explained in section 2.2.1.

$$W_{shaft} = \eta_{filter} \cdot W_{filter} = 0.85 \cdot 0.002\,[kW] \cdot 0.5\,[h] \cdot \frac{3600}{1}\left[\frac{kJ}{kWh}\right] = 3.06\,kJ$$

There are no chemical reactions, meaning that:

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

Therefore:

$$Q_{int} = -W_{shaft} = -3.06\,kJ$$

Table 26. Energy contributions for the second filtration step in lignin extraction process.

Energy contributions	Filtration 2
$(m_k \cdot h_k)_{in}$ [kJ]	0
$(m_k \cdot h_k)_{out}$ [kJ]	0
Q_{int} [kJ]	-3.06
W_{shaft} [kJ]	3.06
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0;\ -3.06 + 3.06 = 0$$

Washing

The process takes place at room temperature, meaning that all the inlet and outlet streams are at 298 K, reference temperature.

$$\sum_k (m_k \cdot h_k)_{in} = \sum_k (m_k \cdot h_k)_{out} = 0$$

Washing is done manually, which implies that there is no mechanical power.

$$W_{shaft} = 0$$

There are no chemical reactions, meaning that:

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

Therefore:

$$Q_{int} = 0$$

Table 27. Energy contributions for the washing step in lignin extraction process.

Energy contributions	Washing
$(m_k \cdot h_k)_{in}$ [kJ]	0
$(m_k \cdot h_k)_{out}$ [kJ]	0
Q_{int} [kJ]	0
W_{shaft} [kJ]	0
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + \mathrm{Q}_{int} + \mathrm{W}_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0; 0 = 0$$

Drying

In drying step, the inlet streams are at room temperature, which means that:

$$\sum_k (m \cdot h_k)_{in} = 0$$

Lignin and sulfuric acid leaves system at an unknown temperature. It is assumed that the temperature is 373 K, a temperature sufficient to evaporate the sulfuric acid used for cleaning.

$$\sum_k (m_k \cdot h_k)_{out} = \left[\left(m_{lignin}\right)_1 \cdot C_{P,lignin,1} + \left(m_{H_2SO_4}\right)_{14a} \cdot C_{P,H_2SO_4,14a}\right] \cdot \left(T_{14a} - T_{ref}\right) + \left(m_{H_2SO_4}\right)_{14a} \cdot \lambda_{H_2SO_4}$$
$$= [1.54 \cdot 25 + 4.46 \cdot 31.18] \cdot (373 - 298) + 31.18 \cdot 2250 = 83.47\ kJ$$

Sulfuric acid solution is evaporated. The evaporation heat used is the same as water, because the solution is mostly constituted by water.

Dryer do not generate mechanical power into the system. Therefore:

$$W_{shaft} = 0$$

There are not chemical reactions.

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

The heat generated by the dryer should satisfy the following equation.

$$Q_{int} = \sum_k (m_k \cdot h_k)_{out} = 83.47\ kJ$$

Table 28. Energy contributions for the drying step in lignin extraction process.

Energy contributions	Drying
$(m_k \cdot h_k)_{in}$ [kJ]	0
$(m_k \cdot h_k)_{out}$ [kJ]	83.47

Energy contributions	Drying
Q_{int} [kJ]	83.47
W_{shaft} [kJ]	0
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + \mathrm{Q}_{int} + \mathrm{W}_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0;\ -83.47 + 83.47 = 0$$

Rubber functionalisation

Sonication

In sonication step, all the compounds are introduced at room temperature, and leave the device at the same temperature. It means that the following results are obtained:

$$\sum_k (m_k \cdot h_k)_{in} = \sum_k (m_k \cdot h_k)_{out} = 0$$

Also, there are no chemical reactions.

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

During sonicating, mechanical power is generated in the system. An efficiency of 85% is considered, as explained in section 2.2.1. The power of the system is provided by the partners.

$$W_{shaft} = \eta_{sonicator} \cdot W_{sonicator} = 0.85 \cdot 0.1\ [kW] \cdot 0.33\ [h] \cdot \frac{3600}{1} \left[\frac{kJ}{kWh}\right] = 100.98\ kJ$$

Therefore:

$$Q_{int} = -W_{shaft} = -100.98\ kJ$$

Table 29. Energy contributions for the sonication step in rubber functionalisation process.

Energy contributions	Sonication
$(m_k \cdot h_k)_{in}$ [kJ]	0
$(m_k \cdot h_k)_{out}$ [kJ]	0
Q_{int} [kJ]	-100.98
W_{shaft} [kJ]	100.98
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0;\ -100.98 + 100.98 = 0$$

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Heating

Heating step takes place in an oven. The materials enter at room temperature, and leaves the oven at 453 K, according to the data provided by the partners.

$$\sum_k (m_k \cdot h_k)_{in} = 0$$

$$\sum_k (\mathrm{m}_k \cdot h_k)_{out} = \left[(m_{rubber})_{3b} \cdot C_{P,rubber,3b} + \left(m_{H_2O}\right)_{3b} \cdot C_{P,DES,3b}\right] \cdot (T_{3b} - T_{ref})$$

$$= 190\ \frac{J}{mol \cdot K} \cdot \frac{1}{86.07} \frac{mol}{g} \cdot 2000\ g + 1.08\ \frac{J}{g \cdot K} \cdot 100\ g = 701.07\ kJ$$

Heat capacity of DES is found in bibliography [24]. Its molar mass has been calculated knowing that DES is made up of chlorine chloride and urea in a 1:2 ratio.

Heat capacity of rubber crumb has also been found in literature [25].

$$C_{P,lignin} = 190\ \frac{J}{mol \cdot K}$$

$$M_{DES} = 86.07\ \frac{g}{mol}$$

$$C_{P,rubber\ crumb} = 1.08\ \frac{J}{g \cdot K}$$

During this step there are not chemical reactions or phase changes, since the solvent is a deep eutectic solvent, and one of its characteristics is that they are non-volatile.

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

Therefore:

$$Q_{int} = \sum_k (m_k \cdot h_k)_{out} = 701.07\ kJ$$

Table 30. Energy contributions for the heating step in rubber functionalisation process.

Energy contributions	Heating
$(m_k \cdot h_k)_{in}$ [kJ]	0
$(m_k \cdot h_k)_{out}$ [kJ]	701.07
Q_{int} [kJ]	701.07
W_{shaft} [kJ]	0
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0;\ -701.07 + 701.07 = 0$$

Filtration

In filtration step, compounds enter the system at the same temperature that they leave in heating step, meaning that:

$$\sum_k (m_k \cdot h_k)_{out,heating} = \sum_k (m_k \cdot h_k)_{in,filtration} = 701.07\ kJ$$

The temperature at which they leave the system is room temperature, which implies:

$$\sum_k (m_k \cdot h_k)_{out} = 0$$

There is no data about how filtration is done, and it is assumed that the process is done with a Büchner funnel. It is assumed that the filtration requires 2 W, as in lignin extraction process, and the process takes place in 60 minutes. The mechanical power generated in the system is assumed to have an efficiency of 85%, as explained in section 2.2.1.

$$W_{shaft} = \eta_{filter} \cdot W_{filter} = 0.85 \cdot 0.002\ [kW] \cdot 1\ [h] \cdot \frac{3600}{1} \left[\frac{kJ}{kWh}\right] = 6.12\ kJ$$

There are no chemical reactions:

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

Therefore:

$$Q_{int} = -W_{shaft} - \sum_k (m_k \cdot h_k)_{in} = -707.19\ kJ$$

Table 31. Energy contributions for the filtration step in rubber functionalisation process.

Energy contributions	Filtration
$(m_k \cdot h_k)_{in}$ [kJ]	701.07
$(m_k \cdot h_k)_{out}$ [kJ]	0
Q_{int} [kJ]	-707.19
W_{shaft} [kJ]	6.12
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0;\ 701.07 - 707.19 + 6.12 = 0$$

Rubber panel production

Compounding

Compounding step stars at room temperature, and no devices for cooling or heating are used. Therefore:

$$\sum_k (m_k \cdot h_k)_{in} = 0$$

Even though, during the process, heat is generated, and the outlet streams are at 313 K.

$$\begin{aligned}\sum_k (m_k \cdot h_k)_{out} = {} & \Big[\big(m_{lignin}\big)_6 \cdot C_{P,lignin,6} + (m_{\text{devulcanised rubber}})_6 \cdot C_{P,devulcanised\ rubber,6} + (m_{\text{rubber crumb}})_6 \cdot C_{P,rubber\ crumb,6} \\ & + (m_{\text{ZnO}})_6 \cdot C_{P,ZnO,6} + (m_{Stearic\ acid})_6 \cdot C_{P,Stearic\ acid,6} + (m_{MBTS-75})_6 \cdot C_{P,MBTS-75,6} + \big(m_{Mesh\ sulphur}\big)_6 \\ & \cdot C_{P,Mesh\ sulphur,6}\Big] \cdot \big(T_6 - T_{ref}\big) \\ & + \Big[\big(m_{lignin}\big)_5 \cdot C_{P,lignin,5} + (m_{\text{devulcanised rubber}})_5 \cdot C_{P,devulcanised\ rubber,5} + (m_{\text{rubber crumb}})_5 \\ & \cdot C_{P,rubber\ crumb,5} + (\dot{m}_{\text{ZnO}})_5 \cdot C_{P,ZnO,5} + (m_{Stearic\ acid})_5 \cdot C_{P,Stearic\ acid,5} + (m_{MBTS-75})_5 \cdot C_{P,MBTS-75,5} \\ & + \big(\dot{m}_{Mesh\ sulphur}\big)_5 \cdot C_{P,Mesh\ sulphur,5}\Big] \cdot \big(T_5 - T_{ref}\big) \\ & = [1.54 \cdot 1.25 + 1.08 \cdot 4 + 1.08 \cdot 1 + 0.49 \cdot 0.25 + 1.76 \cdot 0.05 + 0.57 \cdot 0.03 + 0.73 \cdot 0.13] \cdot (313 - 298) \\ & + [1.54 \cdot 23.75 + 1.08 \cdot 76 + 1.08 \cdot 19 + 0.49 \cdot 4.75 + 1.76 \cdot 0.95 + 0.57 \cdot 0.48 + 0.73 \cdot 2.38] \cdot (313 - 298) \\ & = \ 2.29\ kJ\end{aligned}$$

Specific heats for the components were found in bibliography. For the values that were expressed in $\frac{J}{mol*K}$, they were divided by its molar mass to obtain the desired units expressed in $\frac{J}{g \cdot K}$. For devulcanized and natural rubber, the value of heat capacity is the same, as there is not a significant different between them. For MBTS-75, the value of heat capacity corresponds to a similar substance, such as benzothiazole, as there is no exact data about MBTS-75.

$C_{P,lignin} = 1.54\ \frac{J}{g \cdot K}$ [19]

$C_{P,devulcanised\ rubber} = Cp_{rubber\ crumb} = 1.08\ \frac{J}{g \cdot K}$ [25]

$C_{P,ZnO} = 0.494\ \frac{J}{g \cdot K}$ [26]

$C_{P,Stearic\ acid} = 1.76\ \frac{J}{g \cdot K}$ [21]

$C_{P,MBTS-75} = 0.494\ \frac{J}{g \cdot K}$ [21]

$C_{P,Mesh\ sulphur} = 0.72\ \frac{J}{g \cdot K}$ [21]

There are not any chemical reactions.

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

The mixer generates mechanical power into the system. An efficiency of 85% is considered, as explained in section 2.2.1. Data about the power requirements of the device and the time it takes are provided by the partners.

$$W_{shaft} = \eta_{mixer} \cdot W_{mixer} = 0.85 \cdot 0.313\ [kW] \cdot 0.117\ [h] \cdot \frac{3600}{1}\left[\frac{kJ}{kWh}\right] = 112.06\ kJ$$

Therefore:

$$Q_{int} = -W_{shaft} + \sum_k (m_k \cdot h_k)_{out} = -701090$$

Table 32. Energy contributions for the compounding step in rubber panel production process.

Energy contributions	Compounding
$(m_k \cdot h_k)_{in}$ [kJ]	0
$(m_k \cdot h_k)_{out}$ [kJ]	2.29
Q_{int} [kJ]	-109.77
W_{shaft} [kJ]	112.06
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0;\ -2.29 - 109.77 + 112.06 = 0$$

Cooling

Cooling is done at ambient temperature, but the initial temperature of the compounds is 313 K, as they were heated in the previous step. That means:

$$\sum_k (m_k \cdot h_k)_{out} = 0$$

$$\begin{aligned}\sum_k (\dot{m}_k \cdot h_k)_{in} = & \Big[\left(m_{lignin}\right)_6 \cdot C_{P,lignin,6} + (m_{\text{devulcanised rubber}})_6 \cdot C_{P,devulcanised\ rubber,6} + (m_{\text{rubber crumb}})_6 \cdot C_{P,rubber\ crumb,6} \\ & + (m_{\text{ZnO}})_6 \cdot C_{P,ZnO,6} + (m_{Stearic\ acid})_6 \cdot C_{P,Stearic\ acid,6} + (m_{MBTS-75})_6 \cdot C_{P,MBTS-75,6} + \left(m_{Mesh\ sulphur}\right)_6 \\ & \cdot C_{P,Mesh\ sulphur,6}\Big] \cdot \left(T_6 - T_{ref}\right) \\ & = [1.54 \cdot 23.75 + 1.08 \cdot 76 + 1.08 \cdot 19 + 0.49 \cdot 4.75 + 1.76 \cdot 0.95 + 0.57 \cdot 0.48 + 0.73 \cdot 2.38] \cdot (313 - 298) \\ & = \ 2.18\ kJ\end{aligned}$$

Also, there are not any chemical reactions.

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

There is no mechanical power involved in this step.

$$W_{shaft} = 0$$

Then:

$$Q_{int} = -\sum_k (m_k \cdot h_k)_{in} = -2.18\ kJ$$

Table 33. Energy contributions for the cooling step in rubber panel production process.

Energy contributions	Cooling
$(m_k \cdot h_k)_{in}$ [kJ]	2.18

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Energy contributions	Cooling
$(m_k \cdot h_k)_{out}$ [kJ]	0
Q_{int} [kJ]	-2.18
W_{shaft} [kJ]	0
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0;\ 2.18 - 2.18 = 0$$

Cutting

The entire step takes place at ambient temperature, meaning that:

$$\sum_k (m_k \cdot h_k)_{in} = \sum_k (m_k \cdot h_k)_{out} = 0$$

Also, there are not any chemical reactions, and no mechanical power is used in the step, as the process is done manually.

$$W_{shaft} = 0$$

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

Table 34. Energy contributions for the cutting step in rubber panel production process.

Energy contributions	Cutting
$(m_k \cdot h_k)_{in}$ [kJ]	0
$(m_k \cdot h_k)_{out}$ [kJ]	0
Q_{int} [kJ]	0
W_{shaft} [kJ]	0
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0; 0 = 0$$

Compression moulding

Compression moulding is done with a press. Data about the energy consumption of the press is provided by the partners. During the compression, the piece is heated, but as there is no data about the heat consumption, it is assumed that the power data provided includes also the heating of the piece. The mechanical power generated in the system is assumed to have an efficiency of 85%, as explained in section 2.2.1.

$$W_{shaft} = \eta_{press} \cdot W_{press} = 0.85 \cdot 0.283\,[kW] \cdot 0.5\,[h] \cdot \frac{3600}{1}\left[\frac{kJ}{kWh}\right] = 433\ kJ$$

The process starts at ambient temperature, and after the pressing ends, the sample is cooled. There is no data about how the samples are cooled or the power that it consumes, so it is assumed that the cooling is done with cooling water, which does not generate any mechanical power into the system. As the inlet and outlet streams are at ambient temperature, the following is obtained.

$$\sum_k (m_k \cdot h_k)_{in} = \sum_k (m_k \cdot h_k)_{out} = 0$$

There are no chemical reactions, meaning that:

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

Therefore:

$$Q_{int} = -W_{shaft} = 433\ kJ$$

Table 35. Energy contributions for the compression moulding step in rubber panel production process.

Energy contributions	Compression moulding
$(m_k \cdot h_k)_{in}$ [kJ]	0
$(m_k \cdot h_k)_{out}$ [kJ]	0
Q_{int} [kJ]	-433
W_{shaft} [kJ]	433
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0;\ -433 + 433 = 0$$

Machining

Machining step takes place at ambient temperature, meaning that:

$$\sum_k (m_k \cdot h_k)_{in} = \sum_k (m_k \cdot h_k)_{out} = 0$$

Also, there are not any chemical reactions, and no mechanical power is used in the step, as the process is done manually.

$$W_{shaft} = 0$$

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

$$Q_{int} = 0$$

Table 36. Energy contributions for the machining step in rubber panel production process.

Energy contributions	Machining
$(m_k \cdot h_k)_{in}$ [kJ]	0
$(m_k \cdot h_k)_{out}$ [kJ]	0
Q_{int} [kJ]	0
W_{shaft} [kJ]	0
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0; 0 = 0$$

Exergy balance

Exergy balances are developed following a similar approach to energy balances. In this case, the equation that describes exergy balance is the one that follows:

$$\sum \left(1 - \frac{T_0}{T}\right) Q_{int} + [W - P_0(V_2 - V_1)] + \sum (m_k \cdot \psi)_{in} - \sum (m_k \cdot \psi)_{out} - T_0 S_{gen} = \Delta X_{sys}$$

Even though the process is not steady state, it is considered that there is no accumulation, as it is insignificant, meaning that:

$$\Delta X_{sys} = 0$$

Also, there are not changes in volume, which implies the following.

$$P_0(V_2 - V_1) = 0$$

For all the processes that comprise WP3, the equation used is the one that follows.

$$\sum \left(1 - \frac{T_0}{T}\right) Q_{int} + W + \sum (m_k \cdot \psi)_{in} - \sum (m_k \cdot \psi)_{out} - T_0 S_{gen} = 0$$

In all the processes, kinetic and potential energy are considered negligible.

$$g z_k = \frac{{c_k}^2}{2} = 0$$

Lignin extraction

Pulping

Assuming the considerations made in the energy balance and the results obtained, exergy terms in pulping step can be computed. The compounds are introduced at room temperature, and inside the reactor, they are heated to 448 K, which is the temperature of the outlet stream.

$$\sum (m_k \cdot \psi)_{in} = 0$$

$$\left(1-\frac{T_0}{T}\right)Q_{int}=\left(1-\frac{298}{448}\right)\cdot(-33288)=-11145\ kJ$$

The temperature of the compounds that enter the system room temperature (298 K), which is the same as the reference temperature. Therefore:

$$\begin{aligned}\sum(m_k\cdot\psi)_{out}=&\Big[\left(m_{lignin}\right)_{3a}\cdot C_{P,lignin,3a}+(m_{\text{cellulose}})_{3a}\cdot C_{P,cellulose,3a}+(m_{\text{hemicellulose}})_{3a}\cdot C_{P,hemicellulose,3a}\\&+(m_{\text{other subs}})_{3a}\cdot C_{P,other\ subs,3a}+(m_{NaOH})_{3a}\cdot C_{P,NaOH,3a}+\left(m_{Na_2S}\right)_{3a}\cdot C_{P,Na_2S,3a}+\left(m_{H_2O}\right)_{3a}\cdot C_{P,H_2O,3a}\Big]\\&\cdot\left[\left(T_{3a}-T_{ref}\right)-T_{ref}\cdot ln\frac{T_{3a}}{T_{ref}}\right]\\&=[1.54\cdot 33.35+1.21\cdot 58.36+1.31\cdot 30.57+0.95\cdot 16.65+1.75\cdot 23.61+1.18\cdot 6.94+4.46\cdot 687.93]\\&\cdot\left[448-298-298\cdot ln\frac{448}{298}\right]=\ 93.85\ kJ\end{aligned}$$

Specific heat for the components were found in bibliography and presented in the energy balance.

$$W\ =W_{shaft}=33782\ kJ$$

Therefore:

$$T_0S_{gen}=\sum\left(1-\frac{T_0}{T}\right)Q_{int}+W+\sum(m_k\cdot\psi)_{in}-\sum(m_k\cdot\psi)_{out}=22543.15\ kJ$$

Table 37. Exergy contributions for the pulping step in lignin extraction process.

Exergy contributions	Pulping
$(m_k\cdot h_k)_{in}$ [kJ]	0
$(m_k\cdot h_k)_{out}$ [kJ]	93.85
Q_{int} [kJ]	-11145
W_{shaft} [kJ]	33782
T_0S_{gen} [kJ]	22543.15

$$\sum(m_k\cdot\psi)_{in}-\sum(m_k\cdot\psi)_{out}+\sum\left(1-\frac{T_0}{T}\right)Q_{int}+W-T_0S_{gen}=0;\ -93.85-11145+33782-22543.15=0$$

Filtration 1

In the first filtration step, the exergy term for the inlet mass flows is the same as the outlet term for mass flows in the previous step, which means:

$$\sum(m_k\cdot\psi)_{in}=\ 93.85\ kJ$$

Cellulose and the remaining liquid are removed when reached room temperature, meaning that the only compound that leaves the system at a temperature difference to the reference one is water, as explained in energy analysis.

$$\begin{aligned}\sum(m_k\cdot\psi)_{out}=&\left[\left(\dot{m}_{H_2O}\right)_3\cdot C_{P,H_2O,3}\right]\cdot\left[\left(T_{5a}-T_{ref}\right)-T_{ref}\cdot ln\frac{T_{5a}}{T_{ref}}\right]=[4.46\cdot 358.37]\cdot\left[448-298-298\cdot ln\frac{448}{298}\right]\\&=\ 45.56\ kJ\end{aligned}$$

Work and heat exchange were calculated in energy balance. In this case, the process takes place at room temperature.

$$W = W_{shaft} = 3.06\ kJ$$

$$\left(1-\frac{T_0}{T}\right)Q_{int} = \left(1-\frac{298}{298}\right)\cdot(-257.16) = 0$$

Therefore:

$$T_0S_{gen} = W + \sum(m_k\cdot\psi)_{in} - \sum(m_k\cdot\psi)_{out} = 51.35\ kJ$$

Table 38. Exergy contributions for the first filtration step in lignin extraction process.

Exergy contributions	Filtration 1
$(\mathrm{m}_k\cdot\psi)_{in}$ [kJ]	93.85
$(\mathrm{m}_k\cdot\psi)_{out}$ [kJ]	45.56
$\left(1-\frac{T_0}{T_k}\right)Q_{int}$ [kJ]	0
W [kJ]	3.06
T_0S_{gen} [kJ]	51.35

$$\sum(m_k\cdot\psi)_{in} - \sum(m_k\cdot\psi)_{out} + \sum\left(1-\frac{T_0}{T}\right)Q_{int} + W - T_0S_{gen} = 0;\ 93.85 - 45.56 + 3.06 - 51.35 = 0$$

Acidification

As the entire step takes place at ambient temperature:

$$\sum(m_k\cdot\psi)_{in} = \sum(m_k\cdot\psi)_{out} = 0$$

Work and heat exchange were calculated in energy balance. In this case, the process takes place at room temperature.

$$W = W_{shaft} = 3.06\ kJ$$

$$\left(1-\frac{T_0}{T}\right)Q_{int} = \left(1-\frac{298}{298}\right)\cdot(-3.06) = 0$$

Therefore:

$$T_0S_{gen} = W = 3.06\ kJ$$

Table 39. Exergy contributions for the acidification step in lignin extraction process.

Exergy contributions	Acidification
$(\mathrm{m}_k\cdot\psi)_{in}$ [kJ]	0
$(\mathrm{m}_k\cdot\psi)_{out}$ [kJ]	0
$\left(1-\frac{T_0}{T_k}\right)Q_{int}$ [kJ]	0

Exergy contributions	Acidification
W [kJ]	3.06
T_0S_{gen} [kJ]	3.06

$$\sum(m_k \cdot \psi)_{in} - \sum(m_k \cdot \psi)_{out} + \sum\left(1 - \frac{T_0}{T}\right) Q_{int} + W - T_0S_{gen} = 0;\ 3.06 - 3.06 = 0$$

Filtration 2

The second filtration takes place at room temperature, meaning that all the inlet and outlet streams are at 298 K, reference temperature.

$$\sum(m_k \cdot \psi)_{in} = \sum(m_k \cdot \psi)_{out} = 0$$

Work and heat exchange were calculated in energy balance. In this case, the process takes place at room temperature.

$$W = W_{shaft} = 3.06\ kJ$$

$$\left(1 - \frac{T_0}{T}\right) Q_{int} = \left(1 - \frac{298}{298}\right) \cdot (-3.06) = 0$$

Therefore:

$$T_0S_{gen} = W = 3.06\ kJ$$

Table 40. Exergy contributions for the second filtration step in lignin extraction process.

Exergy contributions	Filtration 2
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	0
$(\mathrm{m}_k \cdot \psi)_{out}$ [kJ]	0
$\left(1 - \frac{T_0}{T_k}\right) Q_{int}$ [kJ]	0
W [kJ]	3.06
T_0S_{gen} [kJ]	3.06

$$\sum(m_k \cdot \psi)_{in} - \sum(m_k \cdot \psi)_{out} + \sum\left(1 - \frac{T_0}{T}\right) Q_{int} + W - T_0S_{gen} = 0;\ 3.06 - 3.06 = 0$$

Washing

The process takes place at room temperature, meaning that all the inlet and outlet streams are at 298 K, reference temperature.

$$\sum(m_k \cdot \psi)_{in} = \sum(m_k \cdot \psi)_{out} = 0$$

Washing is done manually, which implies that there is no mechanical power.

$$W = W_{shaft} = 0$$

There is no heat exchange during this step.

$$\left(1-\frac{T_0}{T}\right)Q_{int} = \left(1-\frac{298}{298}\right)\cdot(0) = 0$$

Therefore:

$$T_0 S_{gen} = 0$$

Table 41. Exergy contributions for the washing step in lignin extraction process.

Exergy contributions	Washing
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	0
$(\mathrm{m}_k \cdot \psi)_{out}$ [kJ]	0
$\left(1-\frac{T_0}{T_k}\right)Q_{int}$ [kJ]	0
W [kJ]	0
$T_0 S_{gen}$ [kJ]	0

$$\sum(m_k\cdot\psi)_{in} - \sum(m_k\cdot\psi)_{out} + \sum\left(1-\frac{T_0}{T}\right)Q_{int} + W - T_0 S_{gen} = 0; 0 = 0$$

Drying

In drying step, the inlet streams are at room temperature, which means that:

$$\sum(m_k\cdot\psi)_{in} = 0$$

Lignin and sulfuric acid leaves system at an unknown temperature. It is assumed that the temperature is 373 K, a temperature sufficient to evaporate the sulfuric acid used for cleaning.

$$\sum_k(\dot{m}_k\cdot h_k)_{out} = \left[(\dot{m}_{lignin})_1\cdot C_{P,lignin,1} + (\dot{m}_{H_2SO_4})_{14a}\cdot C_{P,H_2SO_4,14a}\right]\cdot\left[(T_{14a}-T_{ref}) - T_{ref}\cdot ln\frac{T_{14a}}{T_{ref}}\right]$$
$$= [1.54\cdot 25 + 4.46\cdot 31.18]\cdot\left[373-298-298\cdot ln\frac{373}{298}\right] = 1.44\ kJ$$

There is no mechanical power generated in this step.

$$W = W_{shaft} = 0$$

Heat generated was calculated in energy balance, and the following result is obtained:

$$\left(1-\frac{T_0}{T}\right)Q_{int} = \left(1-\frac{298}{373}\right)\cdot(83.47) = 16.78\ kJ$$

Therefore:

$$T_0 S_{gen} = \sum\left(1-\frac{T_0}{T}\right)Q_{int} - \sum(m_k\cdot\psi)_{out} = 15.34\ kJ$$

Table 42. Exergy contributions for the drying step in lignin extraction process.

Exergy contributions	Drying
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	0
$(\mathrm{m}_k \cdot \psi)_{out}$ [kJ]	1.44
$\left(1-\frac{T_0}{T_k}\right) Q_{int}$ [kJ]	16.78
W [kJ]	0
$T_0 S_{gen}$ [kJ]	15.34

$$\sum(m_k \cdot \psi)_{in} - \sum(m_k \cdot \psi)_{out} + \sum\left(1-\frac{T_0}{T}\right) Q_{int} + W - T_0 S_{gen} = 0;\ -1.44 + 16.78 - 15.34 = 0$$

Rubber functionalisation

Sonication

In sonication step, all the compounds are introduced at room temperature, and leave the device at the same temperature. It means that the following results are obtained:

$$\sum(m_k \cdot \psi)_{in} = \sum(m_k \cdot \psi)_{out} = 0$$

During sonicating, mechanical power is generated in the system. It was calculated in energy analysis.

$$W = W_{shaft} = 100.98\ kJ$$

Heat exchange is described as follows, as the process takes place at reference temperature.

$$\left(1-\frac{T_0}{T}\right) Q_{int} = \left(1-\frac{298}{298}\right) \cdot (-100.98) = 0$$

Therefore:

$$T_0 S_{gen} = W = 22543.15\ kJ$$

Table 43. Exergy contributions for the sonication step in rubber functionalisation process.

Exergy contributions	Sonication
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	0
$(\mathrm{m}_k \cdot \psi)_{out}$ [kJ]	0
$\left(1-\frac{T_0}{T_k}\right) Q_{int}$ [kJ]	0
W [kJ]	100.98
$T_0 S_{gen}$ [kJ]	100.98

$$\sum(m_k\cdot\psi)_{in}-\sum(m_k\cdot\psi)_{out}+\sum\left(1-\frac{T_0}{T}\right)Q_{int}+W-T_0S_{gen}=0; 100.98-100-98=0$$

Heating

The materials enter the oven at room temperature, and leaves it at 453 K.

$$\sum(m_k\cdot\psi)_{in}=0$$

$$\sum(m_k\cdot\psi)_{out}=\left[(\dot{m}_{rubber})_{3b}\cdot C_{P,rubber,3b}+\left(\dot{m}_{H_2O}\right)_{3b}\cdot C_{P,DES,3b}\right]\cdot\left[\left(T_{3b}-T_{ref}\right)-T_{ref}\cdot ln\frac{T_{3b}}{T_{ref}}\right]$$
$$=190\,\frac{J}{mol\cdot K}\cdot\frac{1}{86.07}\frac{mol}{g}\cdot 2000\,g+1.08\,\frac{J}{g\cdot K}\cdot 100\,g\cdot\left[453-298-298\cdot ln\frac{453}{298}\right]=136.59\,kJ$$

During this step, no mechanical power is generated.

$$W=W_{shaft}=0$$

Heat exchange is described as follows.

$$\left(1-\frac{T_0}{T}\right)Q_{int}=\left(1-\frac{298}{453}\right)\cdot(701.07)=239.88\,kJ$$

Therefore:

$$T_0S_{gen}=\sum\left(1-\frac{T_0}{T}\right)Q_{int}-\sum(m_k\cdot\psi)_{out}=103.29\,kJ$$

Table 44. Exergy contributions for the heating step in rubber functionalisation process.

Exergy contributions	Heating
$(m_k\cdot\psi)_{in}$ [kJ]	0
$(m_k\cdot\psi)_{out}$ [kJ]	136.59
$\left(1-\frac{T_0}{T_k}\right)Q_{int}$ [kJ]	239.88
W [kJ]	0
T_0S_{gen} [kJ]	103.29

$$\sum(m_k\cdot\psi)_{in}-\sum(m_k\cdot\psi)_{out}+\sum\left(1-\frac{T_0}{T}\right)Q_{int}+W-T_0S_{gen}=0;\ -136.59+239.88-103.29=0$$

Filtration

In this step, compounds enter the system at the same temperature that they leave in the previous step, meaning that:

$$\sum(m_k\cdot\psi)_{in}=136.59\,kJ$$

The temperature at which they leave the system is room temperature, which implies:

$$\sum(m_k \cdot \psi)_{out} = 0$$

Work was calculated in energy balance analysis.

$$W = W_{shaft} = 6.12\ kJ$$

Heat exchange is described as follows, as the process takes place at reference temperature.

$$\left(1 - \frac{T_0}{T}\right) Q_{int} = \left(1 - \frac{298}{298}\right) \cdot (-707.19) = 0$$

Therefore:

$$T_0 S_{gen} = W + \sum(m_k \cdot \psi)_{in} = 142.71\ kJ$$

Table 45. Exergy contributions for the filtration step in rubber functionalisation process.

Exergy contributions	Filtration
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	136.59
$(\mathrm{m}_k \cdot \psi)_{out}$ [kJ]	0
$\left(1 - \frac{T_0}{T_k}\right) Q_{int}$ [kJ]	0
W [kJ]	6.12
$T_0 S_{gen}$ [kJ]	142.71

$$\sum(m_k \cdot \psi)_{in} - \sum(m_k \cdot \psi)_{out} + \sum\left(1 - \frac{T_0}{T}\right) Q_{int} + W - T_0 S_{gen} = 0; 136.59 + 6.12 - 142.71 = 0$$

Rubber panel production

Compounding

Compounding step stars at room temperature, and no devices for cooling or heating are used. Therefore:

$$\sum(m_k \cdot \psi)_{in} = 0$$

Even though, during the process, heat is generated, and the outlet streams are at 313 K.

$$\begin{aligned}\sum(m_k \cdot \psi)_{out} = &\left[\left(\dot{m}_{lignin}\right)_6 \cdot C_{P,lignin,6} + (\dot{m}_{\text{devulcanised rubber}})_6 \cdot C_{P,devulcanised\ rubber,6} + (\dot{m}_{\text{rubber crumb}})_6 \cdot C_{P,rubber\ crumb,6}\right.\\ &+ (\dot{m}_{\text{ZnO}})_6 \cdot C_{P,ZnO,6} + (\dot{m}_{Stearic\ acid})_6 \cdot C_{P,Stearic\ acid,6} + (\dot{m}_{MBTS-75})_6 \cdot C_{P,MBTS-75,6} + \left(\dot{m}_{Mesh\ sulphur}\right)_6\\ &\left.\cdot C_{P,Mesh\ sulphur,6}\right] \cdot \left[\left(T_6 - T_{ref}\right) - T_{ref} \cdot ln\frac{T_6}{T_{ref}}\right]\\ &+ \left[\left(\dot{m}_{lignin}\right)_5 \cdot C_{P,lignin,5} + (\dot{m}_{\text{devulcanised rubber}})_5 \cdot C_{P,devulcanised\ rubber,5} + (\dot{m}_{\text{rubber crumb}})_5\right.\\ &\cdot C_{P,rubber\ crumb,5} + (\dot{m}_{\text{ZnO}})_5 \cdot C_{P,ZnO,5} + (\dot{m}_{Stearic\ acid})_5 \cdot C_{P,Stearic\ acid,5} + (\dot{m}_{MBTS-75})_5 \cdot C_{P,MBTS-75,5}\\ &\left.+ \left(\dot{m}_{Mesh\ sulphur}\right)_5 \cdot C_{P,Mesh\ sulphur,5}\right] \cdot \left[\left(T_5 - T_{ref}\right) - T_{ref} \cdot ln\frac{T_5}{T_{ref}}\right]\\ &= [1.54 \cdot 1.25 + 1.08 \cdot 4 + 1.08 \cdot 1 + 0.49 \cdot 0.25 + 1.76 \cdot 0.05 + 0.57 \cdot 0.03 + 0.73 \cdot 0.13]\\ &\cdot \left[313 - 298 - 298 \cdot ln\frac{313}{298}\right]\\ &+ [1.54 \cdot 23.75 + 1.08 \cdot 76 + 1.08 \cdot 19 + 0.49 \cdot 4.75 + 1.76 \cdot 0.95 + 0.57 \cdot 0.48 + 0.73 \cdot 2.38]\\ &\cdot \left[313 - 298 - 298 \cdot ln\frac{313}{298}\right] = 0.055\ kJ\end{aligned}$$

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The mixer generates mechanical power into the system. It was calculated in energy analysis, as well as heat exchange.

$$W = W_{shaft} = 112.06\ kJ$$

$$\left(1-\frac{T_0}{T}\right)Q_{int} = \left(1-\frac{298}{313}\right)\cdot(-109.77) = -5.26\ kJ$$

Therefore:

$$T_0S_{gen} = \sum\left(1-\frac{T_0}{T}\right)Q_{int} + W - \sum(m_k\cdot\psi)_{out} = 106.75\ kJ$$

Table 46. Exergy contributions for the compounding step in rubber panel production process.

Exergy contributions	Compounding
$(\mathrm{m}_k\cdot\psi)_{in}$ [kJ]	0
$(\mathrm{m}_k\cdot\psi)_{out}$ [kJ]	0.055
$\left(1-\frac{T_0}{T_k}\right)Q_{int}$ [kJ]	-5.26
W [kJ]	112.06
T_0S_{gen} [kJ]	106.75

$$\sum(m_k\cdot\psi)_{in} - \sum(m_k\cdot\psi)_{out} + \sum\left(1-\frac{T_0}{T}\right)Q_{int} + W - T_0S_{gen} = 0; -0.055 - 5.26 + 112.06 - 106.75 = 0$$

Cooling

Cooling is done at ambient temperature, but the initial temperature of the compounds is 313 K. That means:

$$\sum(m_k\cdot\psi)_{out} = 0$$

$$\begin{aligned}\sum(m_k\cdot\psi)_{in} = {} & \left[\left(\dot{m}_{lignin}\right)_6\cdot C_{P,lignin,6} + (\dot{m}_{\text{devulcanised rubber}})_6\cdot C_{P,devulcanised\ rubber,6} + (\dot{m}_{\text{rubber crumb}})_6\cdot C_{P,rubber\ crumb,6}\right.\\ & + (\dot{m}_{\text{ZnO}})_6\cdot C_{P,ZnO,6} + (\dot{m}_{Stearic\ acid})_6\cdot C_{P,Stearic\ acid,6} + (\dot{m}_{MBTS-75})_6\cdot C_{P,MBTS-75,6} + \left(\dot{m}_{Mesh\ sulphur}\right)_6\\ & \left.\cdot C_{P,Mesh\ sulphur,6}\right]\cdot\left[\left(T_6-T_{ref}\right) - T_{ref}\cdot ln\frac{T_6}{T_{ref}}\right]\\ & = [1.54\cdot 23.75 + 1.08\cdot 76 + 1.08\cdot 19 + 0.49\cdot 4.75 + 1.76\cdot 0.95 + 0.57\cdot 0.48 + 0.73\cdot 2.38]\\ & \cdot\left[313 - 298 - 298\cdot ln\frac{313}{298}\right] = 0.053\ kJ\end{aligned}$$

There is no mechanical power involved in this step.

$$W = W_{shaft} = 0$$

$$\left(1-\frac{T_0}{T}\right)Q_{int} = \left(1-\frac{298}{298}\right)\cdot(-2.18) = 0$$

Therefore:

$$T_0S_{gen} = \sum(m_k\cdot\psi)_{in} = 0.053\ kJ$$

Table 47. Exergy contributions for the cooling step in rubber panel production process.

Exergy contributions	Cooling
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	0.053
$(\mathrm{m}_k \cdot \psi)_{out}$ [kJ]	0
$\left(1-\frac{T_0}{T_k}\right) Q_{int}$ [kJ]	0
W [kJ]	0
$T_0 S_{gen}$ [kJ]	0.053

$$\sum (m_k \cdot \psi)_{in} - \sum (m_k \cdot \psi)_{out} + \sum \left(1-\frac{T_0}{T}\right) Q_{int} + W - T_0 S_{gen} = 0; 0.053 - 0.053 = 0$$

Cutting

The entire step takes place at ambient temperature, meaning that:

$$\sum (m_k \cdot \psi)_{in} = \sum (m_k \cdot \psi)_{out} = 0$$

Also, there is not mechanical power used in the step as the process is done manually, and heat exchange is zero.

$$W = W_{shaft} = 0$$

$$\left(1-\frac{T_0}{T}\right) Q_{int} = \left(1-\frac{298}{298}\right) \cdot 0 = 0$$

Therefore:

$$T_0 S_{gen} = 0$$

Table 48. Exergy contributions for the cutting step in rubber panel production process.

Exergy contributions	Cutting
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	0
$(\mathrm{m}_k \cdot \psi)_{out}$ [kJ]	0
$\left(1-\frac{T_0}{T_k}\right) Q_{int}$ [kJ]	0
W [kJ]	0
$T_0 S_{gen}$ [kJ]	0

$$\sum (m_k \cdot \psi)_{in} - \sum (m_k \cdot \psi)_{out} + \sum \left(1-\frac{T_0}{T}\right) Q_{int} + W - T_0 S_{gen} = 0; 0 = 0$$

Compression moulding

In this step, initial and final temperature are ambient temperature.

$$\sum(m_k \cdot \psi)_{in} = \sum(m_k \cdot \psi)_{out} = 0$$

During compression, the piece is heated, and after its moulding, cooling water is used to heat the piece. Work and heat exchange were calculated in energy section.

$$W = W_{shaft} = 433\ kJ$$

The temperature of the moulding is considered as the temperature of the process.

$$\left(1 - \frac{T_0}{T}\right) Q_{int} = \left(1 - \frac{298}{433}\right) \cdot (-433) = -135\ kJ$$

Therefore:

$$T_0 S_{gen} = \sum\left(1 - \frac{T_0}{T}\right) Q_{int} + W = 298\ kJ$$

Table 49. Exergy contributions for the compression moulding step in rubber panel production process.

Exergy contributions	Compression moulding
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	0
$(\mathrm{m}_k \cdot \psi)_{out}$ [kJ]	0
$\left(1 - \frac{T_0}{T_k}\right) Q_{int}$ [kJ]	-135
W [kJ]	433
$T_0 S_{gen}$ [kJ]	298

$$\sum(m_k \cdot \psi)_{in} - \sum(m_k \cdot \psi)_{out} + \sum\left(1 - \frac{T_0}{T}\right) Q_{int} + W - T_0 S_{gen} = 0;\ -135 + 433 - 298 = 0$$

Machining

Machining step takes place at ambient temperature, meaning that:

$$\sum(m_k \cdot \psi)_{in} = \sum(m_k \cdot \psi)_{out} = 0$$

Also, there are not mechanical power involved or heat exchange.

$$W = W_{shaft} = 0$$

$$\left(1 - \frac{T_0}{T}\right) Q_{int} = \left(1 - \frac{298}{298}\right) \cdot 0 = 0$$

Table 50. Exergy contributions for the machining step in rubber panel production process.

Exergy contributions	Machining
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	0

Exergy contributions	Machining
$(m_k \cdot \psi)_{out}$ [kJ]	0
$\left(1-\frac{T_0}{T_k}\right) Q_{int}$ [kJ]	0
W [kJ]	0
$T_0 S_{gen}$ [kJ]	0

$$\sum(m_k \cdot \psi)_{in} - \sum(m_k \cdot \psi)_{out} + \sum\left(1-\frac{T_0}{T}\right) Q_{int} + W - T_0 S_{gen} = 0; 0 = 0$$

3.1.2. Bio-plastic manufacture (WP4)

Mass balance

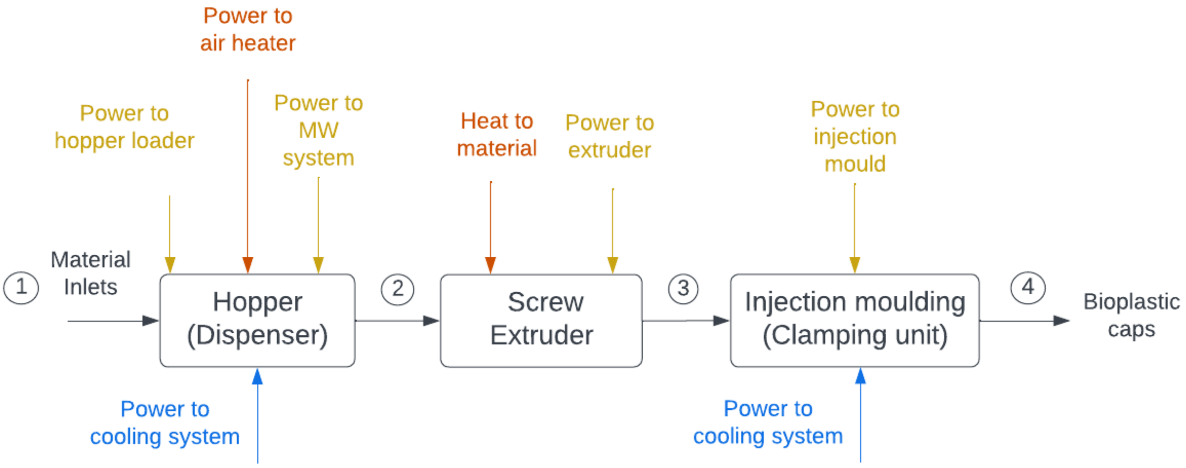

Figure 14. PFD for bio-plastic caps production process.

As described in the methodology, in each step of the process, the following equation must be satisfied. The balances are expressed in grams per batch (g/batch).

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} - \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix} + \begin{pmatrix} Rate\ of \\ generation\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ accumulation\ of\ i \end{pmatrix}$$

Table 51. Mass flows for bio-plastic caps production process.

$\dot{m}_i$ [g/batch]				
Material	**1**	**2**	**3**	**4**
PHBH	6.67	6.67	6.67	6.67
PLA	1.33	1.33	1.33	1.33
Cork	2	2	2	2
Total	10	10	10	10

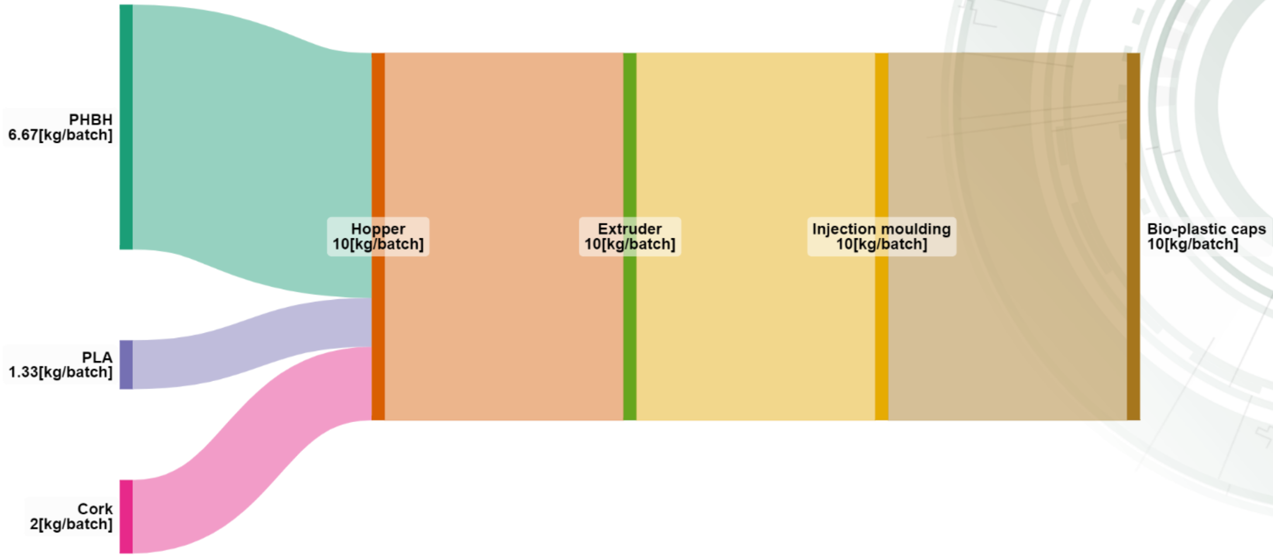

Figure 15. Sankey diagram for bio-plastic caps production.

Dispensation

During this and the subsequent steps there are no accumulation nor chemical reactions. Therefore, all the results are trivial:

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix};\ \dot{m}_1 = \dot{m}_2$$

$$\dot{m}_{1,PHBH} = 6.67 \left[\frac{kg}{batch}\right]\ (E)$$

$$\dot{m}_{1,PLA} = 1.33 \left[\frac{kg}{batch}\right]\ (E)$$

$$\dot{m}_{1,cork} = 2 \left[\frac{kg}{batch}\right]\ (E)$$

$$\dot{m}_{1,PHBH} = \dot{m}_{2,PHBH} = 6.67 \left[\frac{kg}{batch}\right]\ (C)$$

$$\dot{m}_{1,PLA} = \dot{m}_{2,PLA} = 1.33 \left[\frac{kg}{batch}\right]\ (C)$$

$$\dot{m}_{1,cork} = \dot{m}_{2,cork} = 2 \left[\frac{kg}{batch}\right]\ (C)$$

Table 52. Mass flows for dispensation step in bio-plastic caps production process.

$\dot{m}_i$ [g/batch]		
Material	**1 (in)**	**2 (out)**
PHBH	6.67	6.67
PLA	1.33	1.33
Cork	2	2

Total	**10**	**10**

$$\dot{m}_1 = \dot{m}_2; 10 = 10$$

Extrusion

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix}; \dot{m}_2 = \dot{m}_3$$

$$\dot{m}_{2,PHBH} = \dot{m}_{3,PHBH} = 6.67 \left[\frac{kg}{batch}\right] (C)$$

$$\dot{m}_{2,PLA} = \dot{m}_{3,PLA} = 1.33 \left[\frac{kg}{batch}\right] (C)$$

$$\dot{m}_{2,cork} = \dot{m}_{3,cork} = 2 \left[\frac{kg}{batch}\right] (C)$$

Table 53. Mass flows for extrusion step in bio-plastic caps production process.

$\dot{m}_i$ [g/batch]		
Material	**2 (in)**	**3 (out)**
PHBH	6.67	6.67
PLA	1.33	1.33
Cork	2	2
Total	**10**	**10**

$$\dot{m}_2 = \dot{m}_3; 10 = 10$$

Injection moulding

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix}; \dot{m}_3 = \dot{m}_4$$

$$\dot{m}_{3,PHBH} = \dot{m}_{4,PHBH} = 6.67 \left[\frac{kg}{batch}\right] (C)$$

$$\dot{m}_{3,PLA} = \dot{m}_{4,PLA} = 1.33 \left[\frac{kg}{batch}\right] (C)$$

$$\dot{m}_{3,cork} = \dot{m}_{4,cork} = 2 \left[\frac{kg}{batch}\right] (C)$$

Table 54. Mass flows for injection moulding step in bio-plastic caps production process.

$\dot{m}_i$ [g/batch]		
Material	**3 (in)**	**4 (out)**
PHBH	6.67	6.67
PLA	1.33	1.33
Cork	2	2
Total	**10**	**10**

$$\dot{m}_3 = \dot{m}_4; 10 = 10$$

Energy balance

Dispensation

Pellets are preheated before dispensation step, which means that they are dispensed in the hopper at a certain temperature. That temperature is 328 K. The pellets enter and leave at that temperature, because an air heating device is used during the process. Also, a water-cooling device is used to control the temperature.

To conduct the calculation, the mean heat capacity is calculated for the pellets.

$C_{P,PHBH} = 1407 \frac{J}{kg \cdot K}$ [27]

$C_{P,PLA} = 1800 \frac{J}{kg \cdot K}$ [28]

$C_{P,cork} = 1900 \frac{J}{kg \cdot K}$ [29]

$$C_{P,pellet} = C_{P,PHBH} \cdot 0.667 + C_{P,PLA} \cdot 0.133 + C_{P,cork} \cdot 0.2 = 1.558 \frac{kJ}{kg \cdot K}$$

$$\sum_k (m_k \cdot h_k)_{in} = \left[\left(m_{pellet}\right)_1 \cdot C_{P,pellet,1}\right] \cdot \left(T_1 - T_{ref}\right) = [10 \cdot 1.558] \cdot (328 - 298) = 467.4\ kJ$$

$$\sum_k (m_k \cdot h_k)_{out} = \left[\left(m_{pellet}\right)_2 \cdot C_{P,pellet,2}\right] \cdot \left(T_2 - T_{ref}\right) = [10 \cdot 1.558] \cdot (328 - 298) = 467.4\ kJ$$

The hopper does not generate mechanical power in the samples, which means that:

$$W_{shaft} = 0$$

There are not any chemical reactions.

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

Therefore:

$$Q_{int} = 0$$

Table 55. Energy contributions for the dispensation step in bio-plastic caps production process.

Energy contributions	Dispensation
$(m_k \cdot h_k)_{in}$ [kJ]	476.4
$(m_k \cdot h_k)_{out}$ [kJ]	476.4
Q_{int} [kJ]	0
W_{shaft} [kJ]	0
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0; 476.4 - 476.4 = 0$$

Extrusion

During this step, the extruder is heated. The inlet temperature is the outlet temperature from the previous step, in this case, 328 K. In the extruder the samples are heated at 443 K, which is considered as the outlet temperature.

$$\sum_k (m_k \cdot h_k)_{in} = \left[\left(m_{pellet}\right)_2 \cdot C_{P,pellet,2}\right] \cdot \left(T_2 - T_{ref}\right) = [10 \cdot 1.558] \cdot (328 - 298) = 467.4\ kJ$$

$$\sum_k (m_k \cdot h_k)_{out} = \left[\left(m_{pellet}\right)_3 \cdot C_{P,pellet,3}\right] \cdot \left(T_3 - T_{ref}\right) = [10 \cdot 1.558] \cdot (443 - 298) = 2259.1\ kJ$$

The extruder generates mechanical power in the system. An efficiency of 85% is considered, as explained in section 2.2.1.

$$W_{shaft} = \eta_{extruder} \cdot W_{extruder} = 0.85 \cdot 10.95 \left[\frac{kWh}{kg}\right] \cdot\ 10\ [kg] \cdot \frac{3600}{1} \left[\frac{kJ}{kWh}\right] = 335070\ kJ$$

There are not any chemical reactions.

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

Therefore:

$$Q_{int} = -Q_{shaft} - \sum_k (\dot{m}_k \cdot h_k)_{in} + \sum_k (\dot{m}_k \cdot h_k)_{out} = -701090\ kJ$$

Table 56. Energy contributions for the extrusion step in bio-plastic caps production process.

Energy contributions	Extrusion
$(m_k \cdot h_k)_{in}$ [kJ]	476.4
$(m_k \cdot h_k)_{out}$ [kJ]	2259.1
Q_{int} [kJ]	-333287
W_{shaft} [kJ]	335070
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0;\ 476 - 2259 - 33287 + 335070 = 0$$

Injection moulding

During this step, the injection mould is cooled. The inlet temperature is the outlet temperature from the previous step, in this case, 443 K. The outlet temperature is considered to be room temperature.

$$\sum_k (m_k \cdot h_k)_{in} = \left[\left(m_{pellet}\right)_3 \cdot C_{P,pellet,3}\right] \cdot \left(T_3 - T_{ref}\right) = [10 \cdot 1.558] \cdot (443 - 298) = 2259.1\ kJ$$

$$\sum_k (m_k \cdot h_k)_{out} = 0$$

The injection press generates mechanical power in the system. An efficiency of 85% is considered, as explained in section 2.2.1.

$$\dot{W}_{shaft} = \eta_{press} \cdot W_{press} = 0.85 \cdot 4 \left[\frac{kWh}{kg}\right] \cdot 10\,[kg] \cdot \frac{3600}{1}\left[\frac{kJ}{kWh}\right] = 122400\ kJ$$

There are not any chemical reactions.

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

Therefore:

$$Q_{int} = -W_{shaft} - \sum_k (m_k \cdot h_k)_{in} = -124659.1\ kJ$$

Table 57. Energy contributions for the injection moulding step in bio-plastic caps production process.

Energy contributions	Injection moulding
$(m_k \cdot h_k)_{in}$ [kJ]	2259.1
$(m_k \cdot h_k)_{out}$ [kJ]	0
Q_{int} [kJ]	-124659.1
W_{shaft} [kJ]	122400
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0;\ 2259.1 - 124659.1 + 122400 = 0$$

Exergy balance

Dispensation

Pellets are preheated before dispensation step, which means that they are dispensed in the hopper at 328 K. The pellets enter and leave at that temperature, because an air heating device is used during the process.

$$\sum (m_k \cdot \psi)_{in} = \left[\left(\dot{m}_{pellet}\right)_1 \cdot C_{P,pellet,1}\right] \cdot \left[\left(T_1 - T_{ref}\right) - T_{ref} \cdot ln\frac{T_1}{T_{ref}}\right] = [10 \cdot 1.558] \cdot \left[328 - 298 - 298 \cdot ln\frac{328}{298}\right] = 22.06\ kJ$$

$$\sum (m_k \cdot \psi)_{out} = \left[\left(\dot{m}_{pellet}\right)_2 \cdot C_{P,pellet,2}\right] \cdot \left[\left(T_2 - T_{ref}\right) - T_{ref} \cdot ln\frac{T_2}{T_{ref}}\right] = [10 \cdot 1.558] \cdot \left[328 - 298 - 298 \cdot ln\frac{328}{298}\right] = 22.06\ kJ$$

The hopper does not generate mechanical power in the samples, and there is not any heat exchange, which means that:

$$W = W_{shaft} = 0$$

$$\left(1 - \frac{T_0}{T}\right) Q_{int} = \left(1 - \frac{298}{298}\right) \cdot 0 = 0$$

Therefore:

$$T_0S_{gen} = \sum(m_k \cdot \psi)_{in} - \sum(m_k \cdot \psi)_{out} = 0$$

Table 58. Exergy contributions for the dispensation step in bio-plastic caps production process.

Exergy contributions	Dispensation
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	22.06
$(\mathrm{m}_k \cdot \psi)_{out}$ [kJ]	22.06
$\left(1 - \frac{T_0}{T_k}\right) Q_{int}$ [kJ]	0
W [kJ]	0
T_0S_{gen} [kJ]	0

$$\sum(m_k \cdot \psi)_{in} - \sum(m_k \cdot \psi)_{out} + \sum\left(1 - \frac{T_0}{T}\right) Q_{int} + W - T_0S_{gen} = 0; 22.06 - 22.06 = 0$$

Extrusion

During this step, the extruder is heated. The inlet temperature is the outlet temperature from the previous step, in this case, 328 K. In the extruder the samples are heated at 443 K, which is considered as the outlet temperature.

$$\sum(m_k \cdot \psi)_{in} = \left[(\dot{m}_{pellet})_2 \cdot C_{P,pellet,2}\right] \cdot \left[(T_2 - T_{ref}) - T_{ref} \cdot ln\frac{T_2}{T_{ref}}\right] = [10 \cdot 1.558] \cdot \left[328 - 298 - 298 \cdot ln\frac{328}{298}\right] = 22.06\ kJ$$

$$\sum(m_k \cdot \psi)_{out} = \left[(\dot{m}_{pellet})_3 \cdot C_{P,pellet,3}\right] \cdot \left[(T_3 - T_{ref}) - T_{ref} \cdot ln\frac{T_3}{T_{ref}}\right] = [10 \cdot 1.558] \cdot \left[443 - 298 - 298 \cdot ln\frac{443}{298}\right] = 418.32\ kJ$$

The extruder generates mechanical power in the system.

$$W = W_{shaft} = 335070\ kJ$$

Heat exchange was calculated in energy section.

$$\left(1 - \frac{T_0}{T}\right) Q_{int} = \left(1 - \frac{298}{443}\right) \cdot (-333287) = -109089\ kJ$$

Therefore:

$$T_0S_{gen} = \sum\left(1 - \frac{T_0}{T}\right) Q_{int} + W + \sum(m_k \cdot \psi)_{in} - \sum(m_k \cdot \psi)_{out} = 225584\ kJ$$

Table 59. Exergy contributions for the extrusion step in bio-plastic caps production process.

Exergy contributions	Extrusion
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	22.06
$(\mathrm{m}_k \cdot \psi)_{out}$ [kJ]	418.32
$\left(1-\frac{T_0}{T_k}\right) Q_{int}$ [kJ]	-109089
W [kJ]	335070
$T_0 S_{gen}$ [kJ]	225584

$$\sum(m_k \cdot \psi)_{in} - \sum(m_k \cdot \psi)_{out} + \sum\left(1-\frac{T_0}{T}\right) Q_{int} + W - T_0 S_{gen} = 0; 22 - 418 - 109089 + 335070 - 225584 = 0$$

Injection moulding

During this step, the injection mould is cooled. The inlet temperature is the outlet temperature from the previous step, in this case, 443 K. The outlet temperature is considered to be room temperature.

$$\sum(m_k \cdot \psi)_{in} = \left[(\dot{m}_{pellet})_3 \cdot C_{P,pellet,3}\right] \cdot \left[(T_3 - T_{ref}) - T_{ref} \cdot ln\frac{T_3}{T_{ref}}\right] = [10 \cdot 1.558] \cdot \left[443 - 298 - 298 \cdot ln\frac{443}{298}\right] = 418.32\ kJ$$

$$\sum(m_k \cdot \psi)_{out} = 0$$

The injection press generates mechanical power in the system, that was calculated in energy analysis.

$$W = W_{shaft} = 122400\ kJ$$

Also, heat exchange was calculated in energy section.

$$\left(1-\frac{T_0}{T}\right) Q_{int} = \left(1-\frac{298}{298}\right) \cdot (-124659.1) = 0$$

Therefore:

$$T_0 S_{gen} = W + \sum(m_k \cdot \psi)_{in} = 122818.32\ kJ$$

Table 60. Exergy contributions for the injection moulding step in bio-plastic caps production process.

Exergy contributions	Injection moulding
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	418.32
$(\mathrm{m}_k \cdot \psi)_{out}$ [kJ]	0
$\left(1-\frac{T_0}{T_k}\right) Q_{int}$ [kJ]	0
W [kJ]	122400
$T_0 S_{gen}$ [kJ]	122818.32

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$$\sum(m_k \cdot \psi)_{in} - \sum(m_k \cdot \psi)_{out} + \sum\left(1 - \frac{T_0}{T}\right) Q_{int} + W - T_0 S_{gen} = 0; 418.32 + 122400 - 122818.32 = 0$$

3.1.3. Wood composites manufacture (WP5)

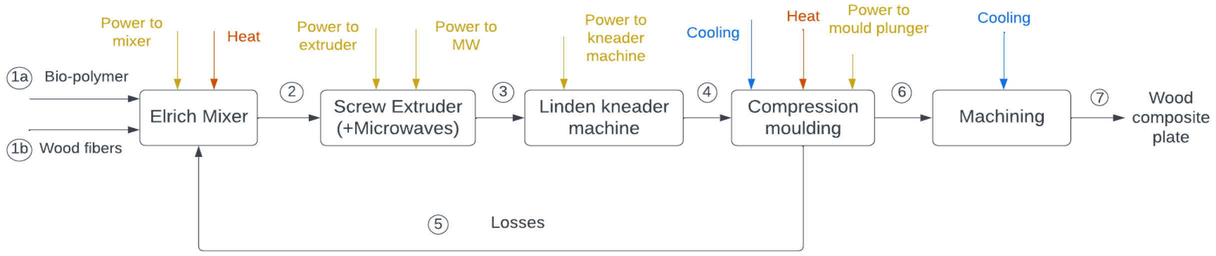

Figure 16. PFD for wood composite production process.

Mass balance

During the production of wood composites there are not chemical reactions nor accumulations. Neither there are any kind of gas emissions. Therefore, the general equation that should be satisfied in all the steps of the process is the following.

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix}$$

Table 61. Mass flows for wood composite production process.

$\dot{m}_i$ [g/batch]							
Material	**1**	**2**	**3**	**4**	**5**	**6**	**7**
Bio-polymer	1000	1091	1091	1091	91	1000	1000
Wood fibres	430	469	469	469	39	430	430
Total	1430	1560	1560	1560	130	1430	1430

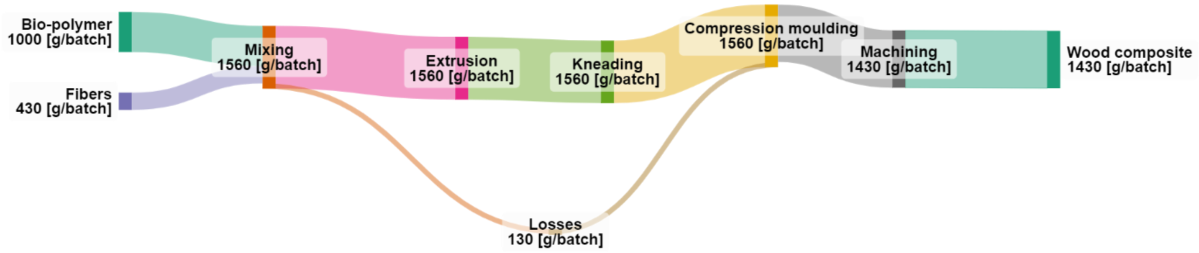

Figure 17. Sankey diagram for wood composite production.

Mixing

In this step, the materials are mixed and heated. Losses from compression moulding step are recovered and use in this step. There are not chemical reactions nor accumulations. Data about the initial mass of bio-polymer and the wood fibres is provided by the partners, as well as data about the percentage recovered in compression moulding step.

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix};\ \dot{m}_1 + \dot{m}_5 = \dot{m}_2$$

$$\dot{m}_{1,bio-polymer} + \dot{m}_{5,bio-polymer} = \dot{m}_{2,bio-polymer}$$

$$\dot{m}_{1,fibres} + \dot{m}_{5,fibres} = \dot{m}_{2,fibres}$$

$$\dot{m}_{1,bio-polymer} = 1000 \left[\frac{g}{batch}\right] (E)$$

$$\dot{m}_{1,fibres} = 430 \left[\frac{g}{batch}\right] (E)$$

Using the data provided by the partners, in compression moulding step, 5/60 are recovered. Meaning that:

$$\dot{m}_{5,bio-polymer} = 91 \left[\frac{g}{batch}\right] (E)$$

$$\dot{m}_{5,fibres} = 39 \left[\frac{g}{batch}\right] (E)$$

$$\dot{m}_{1,bio-polymer} + \dot{m}_{5,bio-polymer} = \dot{m}_{2,bio-polymer} = 1091 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{1,fibres} + \dot{m}_{5,fibres} = \dot{m}_{2,fibres} = 469 \left[\frac{g}{batch}\right] (C)$$

Table 62. Mass flows for mixing step in wood composite production process.

$\dot{m}_i$ [g/batch]			
Material	**1 (in)**	**2 (out)**	**5 (in)**
Bio-polymer	1000	1091	91
Wood fibres	430	469	39
Total	1430	1560	130

$$\dot{m}_1 + \dot{m}_5 = \dot{m}_2;\ 1430 + 130 = 1560$$

Extrusion + Microwaves

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix};\ \dot{m}_2 = \dot{m}_3$$

In extrusion step there are not chemical reactions or accumulations. Losses are considered insignificant. Therefore:

$$\dot{m}_{3,bio-polymer} = \dot{m}_{2,bio-polymer} = 1091 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{3,fibres} = \dot{m}_{2,fibres} = 469 \left[\frac{g}{batch}\right] (C)$$

Table 63. Mass flows for extrusion step in wood composite production process.

$\dot{m}_i$ [g/batch]		
Material	**2 (in)**	**3 (out)**
Bio-polymer	1091	1091
Wood fibres	469	469

Total	1560	1560

$$\dot{m}_2 = \dot{m}_3; 1560 = 1560$$

Kneading

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix}; \ \dot{m}_3 = \dot{m}_4$$

As in the previous step, losses are insignificant.

$$\dot{m}_{3,bio-polymer} = \dot{m}_{4,bio-polymer} = 1091 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{3,fibres} = \dot{m}_{4,fibres} = 469 \left[\frac{g}{batch}\right] (C)$$

Table 64. Mass flows for kneading step in wood composite production process.

$\dot{m}_i$ [g/batch]		
Material	**3 (in)**	**4 (out)**
Bio-polymer	1091	1091
Wood fibres	469	469
Total	1560	1560

$$\dot{m}_2 = \dot{m}_3; 1560 = 1560$$

Compression moulding

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix}; \ \dot{m}_4 = \dot{m}_5 + \dot{m}_6$$

In compression moulding, around 5 g from each 60 g of material will be expelled from the dye and gathered and reused for the next plate. This implies that a fraction of 5/60 of stream 4 is recovered and reuse, which corresponds to stream 5. The losses are recovered and reused in subsequent production to make test components.

$$\dot{m}_{5,bio-polymer} = \frac{5}{60} \cdot \dot{m}_{4,bio-polymer} = 91 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{5,fibres} = \frac{5}{60} \cdot \dot{m}_{4,fibres} = 39 \left[\frac{g}{batch}\right] (C)$$

These masses are the same that were used in mixing step. Therefore, calculations should be correct.

$$\dot{m}_{4,bio-polymer} - \dot{m}_{5,bio-polymer} = \dot{m}_{6,bio-polymer} = 1000 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{4,fibres} - \dot{m}_{5,fibres} = \dot{m}_{6,fibres} = 430 \left[\frac{g}{batch}\right] (C)$$

Table 65. Mass flows for compression moulding step in wood composite production process.

$\dot{m}_i$ [g/batch]			
Material	**4 (in)**	**5 (out)**	**6 (out)**
Bio-polymer	1091	91	1000
Wood fibres	469	39	430
Total	1560	130	1430

$$\dot{m}_4 = \dot{m}_5 + \dot{m}_6; 1560 = 130 + 1430$$

Machining

$$\begin{pmatrix} Rate\ of \\ input\ of\ i \end{pmatrix} = \begin{pmatrix} Rate\ of \\ output\ of\ i \end{pmatrix}; \dot{m}_6 = \dot{m}_7$$

During machining, the sample is cooled, but there are no changes in composition.

$$\dot{m}_{7,bio-polymer} = \dot{m}_{6,bio-polymer} = 1000 \left[\frac{g}{batch}\right] (C)$$

$$\dot{m}_{7,fibres} = \dot{m}_{6,fibres} = 430 \left[\frac{g}{batch}\right] (C)$$

Table 66. Mass flows for machining step in wood composite production process.

$\dot{m}_i$ [g/batch]		
Material	**6 (in)**	**7 (out)**
Bio-polymer	1000	1000
Wood fibres	430	430
Total	1430	1430

$$\dot{m}_6 = \dot{m}_7; 1430 = 1430$$

Energy balance

Mixing

In this first step of the process, both the bio-polymer and the wood fibres are introduced in a mixer, which is heated during the process.

The compounds enter the system at room temperature, and there are not chemical reactions during the process.

$$\sum_k (m_k \cdot h_k)_{in} = 0$$

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

According to the data provided by the partners, the composite comprised of the wood fibres and the bio-polymer leave the mixer at 473 K.

$$\sum_k (m_k \cdot h_k)_{out} = \left[\left(m_{bio-polymer}\right)_2 \cdot C_{P,bio-polymer,2} + (m_{\text{fibres}})_2 \cdot C_{P,fibres,2}\right] \cdot (T_2 - T_{ref})$$

$$= [1.4 \cdot 1091 + 1.34 \cdot 469] \cdot (473 - 298) = \ 377.28\ kJ$$

To estimate heat capacities of the components the following assumptions have been made. The biopolymer is *Tecnaro Arboblend 2241 X*. There is no data about its heat capacity, and it has not been measured experimentally. *Tecnaro Arboblend 2241 X* is comprised of several biopolymers, but the composition in percentage is not revealed. Consequently, to estimate its heat capacity, the average of some of its components has been calculated. For instance, PCL, PET, PLA, nylon 6 [30] and cellulose [21]. The resulting heat capacity of the biopolymer is:

$$C_{P,bio-polymer} = 1.40 \frac{J}{K \cdot g}$$

The wood composite is comprised of the biopolymer and the wood fibres. Wood fibres are C400, C320, C100, FD600/30 and FDB600, from *ARBOCEL*. There is no data available about the heat capacity of these wood fibres, so heat capacity value of wood fibres has been extracted from bibliography [31]. The value found is the average of the values presented in the quoted paper:

$$C_{P,fibres} = 1.34 \frac{J}{K \cdot g}$$

The mixer generates mechanical power in the system. Partners provide data about the consumption of the mixing device. An efficiency of 85% is considered, as explained in section 2.2.1.

$$W_{shaft} = \eta_{mixer} \cdot W_{mixer} = 0.85 \cdot 5\ [kW] \cdot\ 0.5\ [h] \cdot \frac{3600}{1} \left[\frac{kJ}{kWh}\right] = 7650\ kJ$$

Therefore:

$$Q_{int} = -W_{shaft} + \sum_k (m_k \cdot h_k)_{out} = -7326.72\ kJ$$

Table 67. Energy contributions for the mixing step in composite production process.

Energy contributions	Mixing
$(m_k \cdot h_k)_{in}$ [kJ]	0
$(m_k \cdot h_k)_{out}$ [kJ]	377.28
Q_{int} [kJ]	-7272.72
W_{shaft} [kJ]	7650
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0;\ -377.28 - 7272.72 + 7650 = 0$$

Extrusion + Microwaves

The compounds enter the system at 473 K, according to the information provided by the partners. In this step, a microwave system heats the samples, implying that the outlet streams are also at 473 K. Power data is obtained from the specifications sheet of each device.

$$\sum_k (m_k \cdot h_k)_{in} = \left[(m_{bio-polymer})_2 \cdot C_{P,bio-polymer,2} + (m_{\text{fibres}})_2 \cdot C_{P,fibres,2}\right] \cdot (T_2 - T_{ref})$$
$$= [1.4 \cdot 1091 + 1.34 \cdot 469] \cdot (473 - 298) = 377.28\ kJ$$

$$\sum_k (m_k \cdot h_k)_{out} = \left[(m_{bio-polymer})_3 \cdot C_{P,bio-polymer,3} + (m_{\text{fibres}})_3 \cdot C_{P,fibres,3}\right] \cdot (T_3 - T_{ref})$$
$$= [1.4 \cdot 1091 + 1.34 \cdot 469] \cdot (473 - 298) = 377.28\ kJ$$

The compounds enter the system at room temperature, and there are not chemical reactions during the process.

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

The extruder generates mechanical power in the system. Partners provide data about the consumption of the mixing device. An efficiency of 85% is considered, as explained in section 2.2.1.

$$W_{shaft} = \eta_{mixer} \cdot W_{mixer} = 0.85 \cdot 1.5\ [kW] \cdot\ 1.5\ [h] \cdot \frac{3600}{1} \left[\frac{kJ}{kWh}\right] = 6885\ kJ$$

Therefore:

$$Q_{int} = -W_{shaft} + \sum_k (m_k \cdot h_k)_{out} - \sum_k (m_k \cdot h_k)_{in} = -6885\ kJ$$

Table 68. Energy contributions for the extrusion step in composite production process.

Energy contributions	Extrusion
$(m_k \cdot h_k)_{in}$ [kJ]	377.28
$(m_k \cdot h_k)_{out}$ [kJ]	377.28
Q_{int} [kJ]	-6885
W_{shaft} [kJ]	6885
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0; 377.28 - 377.28 - 6885 + 6885 = 0$$

Kneading

In this step, the materials enter the kneader machine at the same temperature they leave the extruder, and no heat is applied during the process. It is assumed that the materials reach ambient temperature by the time they leave the kneader.

$$\sum_k (m_k \cdot h_k)_{out} = 0$$

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$$\sum_k (m_k \cdot h_k)_{in} = \left[\left(m_{bio-polymer}\right)_3 \cdot C_{P,bio-polymer,3} + (m_{\text{fibres}})_3 \cdot C_{P,fibres,3}\right] \cdot (T_3 - T_{ref})$$
$$= [1.4 \cdot 1091 + 1.34 \cdot 469] \cdot (473 - 298) = \ 377.28\ kJ$$

Kneading machine is assumed to have an efficiency of 85%, as explained in section 2.2.1.

$$W_{shaft} = \eta_{kneader} \cdot W_{kneader} = 0.85 \cdot 1.1\ [kW] \cdot 1\ [h] \cdot \frac{3600}{1}\left[\frac{kJ}{kWh}\right] = 3366\ kJ$$

There are no chemical reactions, meaning that:

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

Therefore:

$$Q_{int} = -W_{shaft} - \sum_k (m_k \cdot h_k)_{in} = -3734.28\ kJ$$

Table 69. Energy contributions for the kneading step in composite production process.

Energy contributions	Kneading
$(\ m_k \cdot h_k)_{in}$ [kJ]	377.28
$(m_k \cdot h_k)_{out}$ [kJ]	0
Q_{int} [kJ]	-3734.28
W_{shaft} [kJ]	3366
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0; 377.28 - 3734.28 + 2266 = 0$$

Compression moulding

In compression moulding step, the materials enter the device at room temperature, and they are heated during the entire process. Cooling devices are also used. The outlet temperature is 473 K.

$$\sum_k (m_k \cdot h_k)_{in} = 0$$

$$\sum_k (m_k \cdot h_k)_{out} = \left[\left(m_{bio-polymer}\right)_6 \cdot C_{P,bio-polymer,6} + (m_{\text{fibres}})_6 \cdot C_{P,fibres,6}\right] \cdot (T_6 - T_{ref})$$
$$= [1.4 \cdot 1091 + 1.34 \cdot 469] \cdot (473 - 298) = \ 377.28\ kJ$$

Compression moulding device is assumed to have an efficiency of 85%, as explained in section 2.2.1.

$$W_{shaft} = \eta_{kneader} \cdot W_{kneader} = 0.85 \cdot 10\ [kW] \cdot 0.67\ [h] \cdot \frac{3600}{1}\left[\frac{kJ}{kWh}\right] = 20502\ kJ$$

There are no chemical reactions, meaning that:

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

Therefore:

$$Q_{int} = -W_{shaft} + \sum_k (m_k \cdot h_k)_{out} = -20124.72\ kJ$$

Table 70. Energy contributions for the compression moulding step in composite production process.

Energy contributions	Compression moulding
$(m_k \cdot h_k)_{in}$ [kJ]	0
$(m_k \cdot h_k)_{out}$ [kJ]	377.28
Q_{int} [kJ]	-20124.72
W_{shaft} [kJ]	20502
$\sum \Delta H_R^{Tref}$ [kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0;\ -377.28 - 20124.72 + 20502 = 0$$

Machining

Machining step involves cooling the sample and removing from the moulding step. The final temperature is 298 K, and the initial one is the outlet temperature in compression moulding, which is 473 K.

$$\sum_k (m_k \cdot h_k)_{out} = 0$$

$$\sum_k (m_k \cdot h_k)_{in} = \left[\left(m_{bio-polymer}\right)_6 \cdot C_{P,bio-polymer,6} + (m_{\text{fibres}})_6 \cdot C_{P,fibres,6}\right] \cdot \left(T_6 - T_{ref}\right)$$
$$= [1.4 \cdot 1000 + 1.34 \cdot 430] \cdot (473 - 298) = 345.84\ kJ$$

As it is a manual process and there are not any chemical reactions:

$$W_{shaft} = 0$$

$$\sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0$$

Therefore:

$$Q_{int} = -\sum_k (m_k \cdot h_k)_{in} = -345.84\ kJ$$

Table 71. Energy contributions for the machining step in composite production process.

Energy contributions	Machining
$(m_k \cdot h_k)_{in}$ [kJ]	345.84

Energy contributions	Machining
$(m_k \cdot h_k)_{out}$ [kJ]	0
Q_{int} [kJ]	-345.84
W_{shaft} [kJ]	0
$\sum \Delta H_R^{Tref}$[kJ]	0

$$\sum_k (m_k \cdot h_k)_{in} - \sum_k (m_k \cdot h_k)_{out} + Q_{int} + W_{shaft} + \sum_j \left(\Delta H_j^{Tref} \cdot r_j\right) = 0; 345.84 - 345.84 = 0$$

Exergy balance

Mixing

In this first step of the process, both the bio-polymer and the wood fibres are introduced in a mixer, which is heated to 473 K during the process.

$$\sum (m_k \cdot \psi)_{in} = 0$$

$$\sum (m_k \cdot \psi)_{out} = \left[\left(\dot{m}_{bio-polymer}\right)_2 \cdot C_{P,bio-polymer,2} + (\dot{m}_{\text{fibres}})_2 \cdot C_{P,fibres,2}\right] \cdot \left[\left(T_2 - T_{ref}\right) - T_{ref} \cdot ln\frac{T_2}{T_{ref}}\right]$$
$$= [1.4 \cdot 1091 + 1.34 \cdot 469] \cdot \left[473 - 298 - 298 \cdot ln\frac{473}{298}\right] = \ 80.47\ kJ$$

Mechanical power generated in the system and heat exchange were previously calculated.

$$W\ = W_{shaft} = 7650\ kJ$$

$$\left(1 - \frac{T_0}{T}\right) Q_{int} = \left(1 - \frac{298}{473}\right) \cdot (-7272.72) = -2690.75\ kJ$$

Therefore:

$$T_0 S_{gen} = \sum \left(1 - \frac{T_0}{T}\right) Q_{int} + W - \sum (m_k \cdot \psi)_{out} = 4878.78\ kJ$$

Table 72. Exergy contributions for the mixing step in composite production process.

Exergy contributions	Mixing
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	0
$(\mathrm{m}_k \cdot \psi)_{out}$ [kJ]	80.47
$\left(1 - \frac{T_0}{T_k}\right) \mathrm{Q}_{int}$ [kJ]	-2690.75
W [kJ]	7650
$T_0 S_{gen}$ [kJ]	4878.48

$$\sum (m_k \cdot \psi)_{in} - \sum (m_k \cdot \psi)_{out} + \sum \left(1 - \frac{T_0}{T}\right) Q_{int} + W - T_0 S_{gen} = 0;\ -80.47 - 2690.75 + 7650 - 4878.48 = 0$$

Extrusion + Microwaves

The compounds enter the system at 473 K, according to the information provided by the partners. In this step, a microwave system heats the samples, implying that the outlet streams are also at 473 K. Power data is obtained from the specifications sheet of each device.

$$\sum(m_k \cdot \psi)_{in} = \left[(\dot{m}_{bio-polymer})_2 \cdot C_{P,bio-polymer,2} + (\dot{m}_{\text{fibres}})_2 \cdot C_{P,fibres,2}\right] \cdot \left[(T_2 - T_{ref}) - T_{ref} \cdot ln\frac{T_2}{T_{ref}}\right]$$
$$= [1.4 \cdot 1091 + 1.34 \cdot 469] \cdot \left[473 - 298 - 298 \cdot ln\frac{473}{298}\right] = 80.47\ kJ$$

$$\sum(m_k \cdot \psi)_{out} = \left[(\dot{m}_{bio-polymer})_3 \cdot C_{P,bio-polymer,3} + (\dot{m}_{\text{fibres}})_3 \cdot C_{P,fibres,3}\right] \cdot \left[(T_3 - T_{ref}) - T_{ref} \cdot ln\frac{T_3}{T_{ref}}\right]$$
$$= [1.4 \cdot 1091 + 1.34 \cdot 469] \cdot \left[473 - 298 - 298 \cdot ln\frac{473}{298}\right] = 80.47\ kJ$$

The extruder generates mechanical power in the system. It was calculated in the energy balance, as well as heat exchange.

$$W = W_{shaft} = 6885\ kJ$$

$$\left(1 - \frac{T_0}{T}\right) Q_{int} = \left(1 - \frac{298}{473}\right) \cdot (-6885) = -2547.30\ kJ$$

Therefore:

$$T_0 S_{gen} = \sum\left(1 - \frac{T_0}{T}\right) Q_{int} + W + \sum(m_k \cdot \psi)_{in} - \sum(m_k \cdot \psi)_{out} = 4337.70\ kJ$$

Table 73. Exergy contributions for the extrusion step in composite production process.

Exergy contributions	Extrusion
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	80.47
$(\mathrm{m}_k \cdot \psi)_{out}$ [kJ]	80.47
$\left(1 - \frac{T_0}{T_k}\right) Q_{int}$ [kJ]	-2547.30
W [kJ]	6885
$T_0 S_{gen}$ [kJ]	4337.70

$$\sum(m_k \cdot \psi)_{in} - \sum(m_k \cdot \psi)_{out} + \sum\left(1 - \frac{T_0}{T}\right) Q_{int} + W - T_0 S_{gen} = 0; 80.47 - 80.47 - 2547.3 + 6885 - 4337.7 = 0$$

Kneading

In this step, the materials enter the kneader machine at the same temperature they leave the extruder, and no heat is applied during the process. It is assumed that the materials reach ambient temperature by the time they leave the kneader.

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$$\sum(m_k \cdot \psi)_{out} = 0$$

$$\sum(m_k \cdot \psi)_{in} = \left[\left(\dot{m}_{bio-polymer}\right)_3 \cdot C_{P,bio-polymer,3} + (\dot{m}_{\text{fibres}})_3 \cdot C_{P,fibres,3}\right] \cdot \left[\left(T_3 - T_{ref}\right) - T_{ref} \cdot ln\frac{T_3}{T_{ref}}\right]$$

$$= [1.4 \cdot 1091 + 1.34 \cdot 469] \cdot \left[473 - 298 - 298 \cdot ln\frac{473}{298}\right] = 80.47\ kJ$$

Kneading machine generates mechanical power in the system. It was calculated in the energy balance, as well as heat exchange.

$$W = W_{shaft} = 3366\ kJ$$

$$\left(1 - \frac{T_0}{T}\right) Q_{int} = \left(1 - \frac{298}{298}\right) \cdot (-3734.28) = 0$$

Therefore:

$$T_0 S_{gen} = W + \sum(m_k \cdot \psi)_{in} = 2064.87\ kJ$$

Table 74. Exergy contributions for the kneading step in composite production process.

Exergy contributions	Kneading
$(m_k \cdot \psi)_{in}$ [kJ]	80.47
$(m_k \cdot \psi)_{out}$ [kJ]	0
$\left(1 - \frac{T_0}{T_k}\right) Q_{int}$ [kJ]	0
W [kJ]	3366
$T_0 S_{gen}$ [kJ]	3446.47

$$\sum(m_k \cdot \psi)_{in} - \sum(m_k \cdot \psi)_{out} + \sum\left(1 - \frac{T_0}{T}\right) Q_{int} + W - T_0 S_{gen} = 0; 80.47 + 3366 - 2446.47 = 0$$

Compression moulding

In compression moulding step, the materials enter the device at room temperature, and they are heated during the entire process at 473 K.

$$\sum(m_k \cdot \psi)_{in} = 0$$

$$\sum(m_k \cdot \psi)_{out} = \left[\left(\dot{m}_{bio-polymer}\right)_6 \cdot C_{P,bio-polymer,6} + (\dot{m}_{\text{fibres}})_6 \cdot C_{P,fibres,6}\right] \cdot \left[\left(T_6 - T_{ref}\right) - T_{ref} \cdot ln\frac{T_6}{T_{ref}}\right]$$

$$= [1.4 \cdot 1091 + 1.34 \cdot 469] \cdot \left[473 - 298 - 298 \cdot ln\frac{473}{298}\right] = 80.47\ kJ$$

Compression moulding device generates mechanical work in the system.

$$W = W_{shaft} = 20502\ kJ$$

Heat exchange was calculated in the energy section.

$$\left(1 - \frac{T_0}{T}\right) Q_{int} = \left(1 - \frac{298}{473}\right) \cdot (-20124.72) = -7445.72\ kJ$$

Therefore:

$$T_0 S_{gen} = \sum\left(1-\frac{T_0}{T}\right) Q_{int} + W + \sum(m_k \cdot \psi)_{in} = 12975.81\ kJ$$

Table 75. Exergy contributions for the compression moulding step in composite production process.

Exergy contributions	Compression moulding
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	0
$(\mathrm{m}_k \cdot \psi)_{out}$ [kJ]	80.47
$\left(1-\frac{T_0}{T_k}\right) Q_{int}$ [kJ]	-7445.72
W [kJ]	20502
$T_0 S_{gen}$ [kJ]	12975.81

$$\sum(m_k \cdot \psi)_{in} - \sum(m_k \cdot \psi)_{out} + \sum\left(1-\frac{T_0}{T}\right) Q_{int} + W - T_0 S_{gen} = 0;\ -80.47 - 7445.72 + 20502 - 12975.81 = 0$$

Machining

Machining step involves cooling the sample and removing from the moulding step. The final temperature is 298 K, and the initial one is the outlet temperature in compression moulding, which is 473 K.

$$\sum(m_k \cdot \psi)_{out} = 0$$

$$\sum(m_k \cdot \psi)_{in} = \left[(\dot{m}_{bio-polymer})_6 \cdot C_{P,bio-polymer,6} + (\dot{m}_{\text{fibres}})_6 \cdot C_{P,fibres,6}\right] \cdot \left[(T_6 - T_{ref}) - T_{ref} \cdot ln\frac{T_6}{T_{ref}}\right]$$
$$= [1.4 \cdot 1000 + 1.34 \cdot 430] \cdot \left[473 - 298 - 298 \cdot ln\frac{473}{298}\right] = 73.76\ kJ$$

As it is a manual process there is not mechanical work. Also, there is not heat exchange.

$$W = W_{shaft} = 0$$

$$\left(1-\frac{T_0}{T}\right) Q_{int} = \left(1-\frac{298}{298}\right) \cdot 0 = 0$$

Therefore:

$$T_0 S_{gen} = \sum(m_k \cdot \psi)_{in} = 73.76$$

Table 76. Exergy contributions for the machining step in composite production process.

Exergy contributions	Machining
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	73.76
$(\mathrm{m}_k \cdot \psi)_{out}$ [kJ]	0

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Exergy contributions	Machining
$\left(1-\frac{T_0}{T_k}\right)Q_{int}$ [kJ]	0
W [kJ]	0
T_0S_{gen} [kJ]	73.76

$$\sum(m_k \cdot \psi)_{in} - \sum(m_k \cdot \psi)_{out} + \sum\left(1-\frac{T_0}{T}\right)Q_{int} + W - T_0S_{gen} = 0; 73.76 - 73.76 = 0$$

3.2. Life Cycle Analysis

In order to assess the impact of the different products obtained by the GREEN-LOOP; bio-rubber, bioplastic and wood composites have been selected to represent the use of this project. The value chain for each product obtained are described in Figure 12 for bio-panels, Figure 14 for bioplastic closures, and Figure 16 for the wood composites.

The scope of these PFDs is focused in the manufacturing processes, not the whole value chain including transports, use phase or EoL; since the boundaries (Figure 18) for these first approach analyses will take in-to account only manufacture step, which would be equivalent to “Cradle-to-Gate” analyses, due to it is considered the Raw Materials and the intrinsic average transport in the database used in the Software. Thus, “Cradle-to-Gate” scope has been chosen in order to evaluate the environmental impact of every manufactured component by current and new processes.

These boundaries have been established taking account different cut-off criteria, such as the fact that it is a preliminary analysis (scope of D2.2, and in accordance with the developments performed during the first stage of the project), which will help to focus on where the greatest environmental load is within each of the processes associated with the GREEN-LOOP Project. The main objective is to identify the potential impacts and their relationship with the system and the conditions that can be established in this operation design phase (validation and testing).

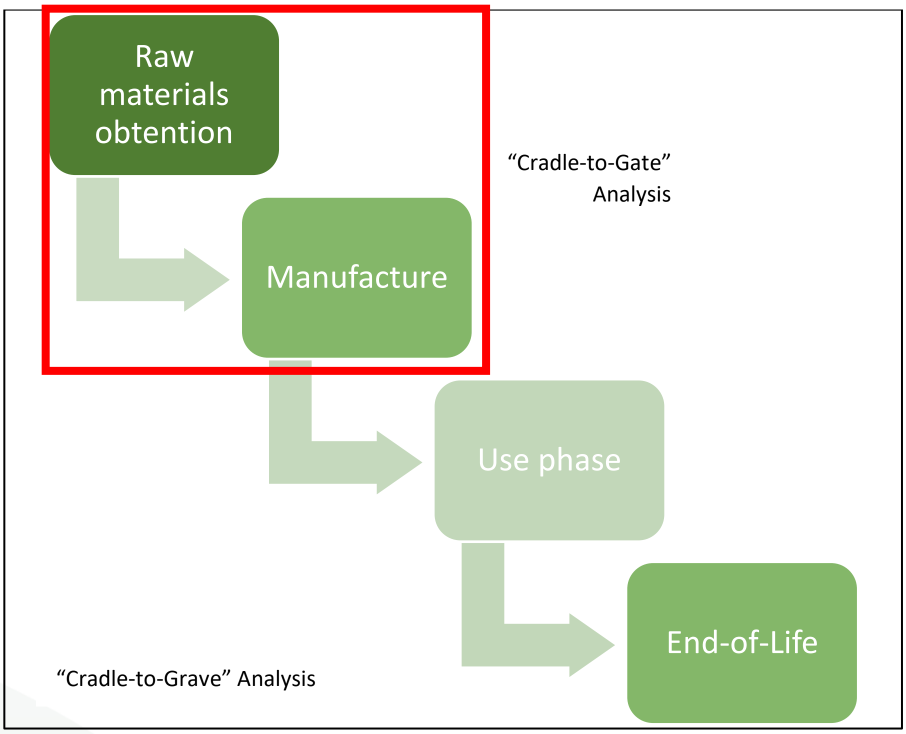

Figure 18. Scope of the analyses of GREEN-LOOP products.

3.2.1. Definition of comparison scenarios

The preliminary LCA has focused on the current process by which the 3 target products are obtained; the rubber panels, the Aluminium-LDPE plastic closures, and the metallic sliding bearings, in addition to the processes developed in the GREEN-LOOP project. In order to the new processes, it will be taken into account two different scenarios for each value chain, 2 scenarios developed in the project and another for benchmarking (current) that represents current option in the market.

The dataset used during the estimation of environmental impacts for the bio-rubber panels in WP3 is shown below. In Table 106, Table 107 and Table 108, in the ANNEX, are collected all the data related with the manufacturing of WP3, but with different scenarios: Lignin recovery step within one 1.8L reactor, BRP1; Lignin recovery step with a 0.8L reactor and a sonicator, BRP2; and the current situation (only the synthetic rubber is used instead of the natural rubber) taking into account the first electricity scenario, due to the fact that data is from lab scale is not comparable in terms of energy consumption with an industrial scale.

WP3 process is shown in Figure 12, according with the value chain for rubber panel production, and the different scenarios are listed below:

- BRP1: bio-rubber panel scenario 1.8L reactor
- BRP2: bio-rubber panel scenario 0.5L reactor + ultrasound sonicator
- Current: current rubber panel

Different assumptions have been made for all the scenarios, as the acid liquor in the lignin recovery:

- It has been assumed to be a very dilute mixture of sulphuric acid and water.
- In the Rubber functionalization step, the 70% of vulcanized rubber crumbs is divided into 70% is Synthetic rubber, 29% is carbon black powder, and 1% of amorphous silicon dioxide introduced in the dataset as silica sand.

- The Deep Eutectic Solvent is a mixture of Choline Chloride (ChCl) and Urea with a ratio of 1 mol ChCl:2 mol Urea, but as there is no existing entry for ChCl, Ammonium Chloride has been introduced as it is a compound of the same family and with a very similar formulation.

- At the final step, the Compounding phase, is used the natural rubber as additive, and in the literature review [32] is accepted to take a natural rubber as an acrylonitrile-butadiene-styrene (ABS) rubber but without styrene in the formulation.

- In the curatives flow, the MBTS-75 (2,2’-Dibenzothiazolyl Disulfide) works as an accelerator, but as in the previous assumption, there is no entry for that particular compound, so a similar and assimilable one has been selected: dimethyl sulphide.

As it was commented above, the second scenario for the WP3 comparative analysis is the same structure as the previous one but changing the energy requirements for the lignin recovery; a 1.8L reactor is substituted for another 0.8L reactor but with an ultrasound sonicator. This change affects the Lignin extraction step, remarked in red in Table 107. As energy consumptions are different, the outputs are different too, so there will be ‘Lignin extraction v1’ and ‘Lignin extraction v2’. The existent of two output from the first step will generate two inputs for the composite production step.

For the current situation – Table 108 - related with the rubber panels manufacturing, the main change that has been made is the use of synthetic virgin rubber instead of natural rubber (acrylonitrile and butadiene).

The dataset used in the WP4 analysis will be collected in Table 109, Table 110 and Table 111; one table for each scenario. The first one is for a composition for olive oil closures with cork and two biopolymers; the second is the same olive oil closure but only made with biopolymers; and the final scenario is the current plastic olive oil closures, which is one of the main materials used nowadays for this purpose.

WP4 value chain is represented in Figure 14, and in the following list are collected the scenarios for this process:

- wCORK: bioplastic closures with cork
- w/oCORK: bioplastic closures without cork
- Current: current plastic closures – aluminium and Low-Density Polyethylene (LDPE)

The raw materials are the only difference between the 3 systems, and how it was mentioned above, the fact that this kind of data is from a laboratory, it is not making sense to compare it with an energy consumption from industry. In the three scenarios, the generation of waste or emissions is not taken into account, although the energy requirements are considered the same.

In relation to the information required for WP5, eight different material compositions have been taken into account. Two of them have only wood and biopolymer in different proportions; five mixtures also have graphite in different amounts; and the last option is the current manufacturing system. The different ratios of mixtures are presented below in Table 77:

Table 77. Mixtures for WP5

Material (%)	MIX1	MIX2	MIX3	MIX4	MIX5	MIX6	MIX7
Wood	50	40	39.6	49.5	48.5	47.5	45
Biopolymer	50	60	59.4	49.5	48.5	47.5	45
Graphite	0	0	1	1	3	5	10

In order to avoid a repetitive representation of tables in this section, a representative table for each type of mix (Table 112, Table 113 and Table 114) has been added in the annex: wood and biopolymer, MIX1; wood, biopolymer and graphite, MIX3; and the current system. This traditional manufacturing will be studied with a copper alloy as a main raw material, due to provide a broad selection of material properties that make them suitable for many bearing applications [33]. As in the previous cases, the energy requirements will be the same for all scenarios. Another point that will be different during the 3 scenarios is the nature of the waste; each waste will be characterised by its raw material, so the final environmental impacts will be different.

The value chain for WP5 is represented in Figure 16, and the different scenarios for this process are collected in the following list:

- MIX1: wood composites with mixture 1 (50% wood – 50% bioplastic)
- MIX3: wood composites with mixture 3 (39,6% wood – 59,4% bioplastic – 1% graphite)
- Current: current metallic sliding bearing (copper alloy)

For three value chains, the functional unit (FU) defined is **1 kg of bio-based manufactured material**; 1kg of bio-rubber for the WP3, 1 kg of bioplastic for WP4, and 1 kg of wood composite for the WP5. Using this value as the functional unit, 1 kg of the corresponding material is also selected for the current manufacturing processes.

3.2.2. Life Cycle Inventories

The different inventories for each scenario from every value chain are explained and described in next sub-sections. It has been explained the inventory differences between scenarios and some assumptions used during the development of these LCIs.

3.2.2.1. Bio-rubber manufacture

The following tables are showing the inventories for three scenarios represented in the WP3, inside the GREEN-LOOP Project. The first column is representing the step represents the step where the inputs/outputs of the second column are located. The third column will contain the value of the analysis introduced in the software, accompanied by the unit of this value. The Figure 12 represents the value chain developed in this section.

In order, Table 78 has the LCI related with the first scenario, bio-rubber panel - BRP1: a 1.8L reactor during ‘Lignin extraction’ step. In the Software, the Eutectic Solvent has a positive and negative value because this mixture remains in the process, neither entering nor leaving. The rest of assumptions are commented during the section 2.3.2, ‘Datasets and computational tools used’. In final step, the bio-rubber panel conformation, the natural rubber works as additives in the process, and as curing agents, the selected materials are zinc oxide, stearic acid, MBTS-75 (as accelerator), and finally, sulphur.

When entering data in SIMAPRO, the three steps are entered separately so that all three steps have the same FU, but in the compounding step, the material balance is adjusted in such a way that the output is 1 kg of material for bio-rubber panels.

Table 78. LCI for WP3-BRP1

	WP3	Quantity	Unit
Lignin extraction 1	**INPUT**		
	Distilled water	35.85	kg
	Sodium sulphide	0.28	kg
	Sodium hydroxide	0.94	kg
	Lignocellulose Biomass	5.56	kg
	Sulfuric Acid 98%	1.10	kg
	OUTPUT		
	Lignin powder	**1**	kg
	WASTE		
	Acid liquor	39.43	kg
	Cellulose rich waste	2.86	kg
	EMISSIONS		
	-		
	ENERGY REQUIREMENTS		
	High-pressure batch reactor	266.54	kWh/kg
Rubber functionalization	**INPUT**		
	Vulcanized rubber crumbs (70% synthetic rubber, 29% carbon black and 1% silica sand)	0.875	kg
		0.3625	kg
		0.0125	kg

	WP3	Quantity	Unit
	Deep Eutectic Solvent	(+/-) 8.330	kg
		(+/-) 16.670	kg
	OUTPUT		
	Devulcanized Rubber (70%)	**1**	kg
	WASTE		
	Waste rubber	2.000	kg
	EMISSIONS		
	-		
	ENERGY REQUIREMENTS		
	Oven 1	14.4	kWh/kg
	Ultrasound equipment	1.32	kWh/kg
	Oven 2	4.8	kWh/kg
Biorubber panel 1	**INPUT**		
	Devulcanized Rubber (70%)	0.696	kg
	Lignin powder	0.218	kg
	Natural rubber	0.104	kg
		0.070	kg
	Low Lead Zinc Oxide	0.044	kg
	Stearic acid	0.009	kg
	MBTS-75	0.004	kg
	300 Mesh Sulphur	0.022	kg
	OUTPUT		
	Bio-rubber panel	**1**	kg
	WASTE		
	Polymer filament	0.108	kg
	EMISSIONS		
	-	-	
	ENERGY REQUIREMENTS		
	Compounding	0.313	kWh/kg
	Compression Moulding	0.283	kWh/kg

In Table 79 is collected all the data related with WP3 too, BRP2, but in this case is different the Energy Requirements from “Lignin extraction” phase: in this case the high-pressure reactor 1.8L is changed by other one with 0.5L of capacity and with an ultrasound sonicator. The energy consumption in these conditions is lower than the previous scenario. Rubber functionalization and Panel conformation are exactly the same processes.

Table 79. LCI for WP3-BRP2

	WP3	Quantity	Unit
Lignin extraction 2	**INPUT**		

	WP3	Quantity	Unit
	Distilled water	35.85	kg
	Sodium sulphide	0.28	kg
	Sodium hydroxide	0.94	kg
	Lignocellulose Biomass	5.56	kg
	Sulfuric Acid 98%	1.10	kg
	OUTPUT		
	Lignin powder	**1**	kg
	WASTE		
	Acid liquor	39.43	kg
	Cellulose rich waste	2.86	kg
	EMISSIONS		
	-		
	ENERGY REQUIREMENTS		
	Ultrasound sonicator	46.86	kWh/kg
	High-pressure batch reactor	134.66	kWh/kg
Rubber functionalization	**INPUT**		
	Vulcanized rubber crumbs (70% synthetic rubber, 29% carbon black and 1% silica sand)	0.875	kg
		0.3625	kg
		0.0125	kg
	Deep Eutectic Solvent	(+/-) 8.330	kg
		(+/-) 16.670	kg
	OUTPUT		
	Devulcanized Rubber (70%)	**1**	kg
	WASTE		
	Waste rubber	2.000	kg
	EMISSIONS		
	-		
	ENERGY REQUIREMENTS		
	Oven 1	14.4	kWh/kg
	Ultrasound equipment	1.32	kWh/kg
	Oven 2	4.8	kWh/kg
Biorubber panel 2	**INPUT**		
	Devulcanized Rubber (70%)	0.696	kg
	Lignin powder	0.218	kg
	Natural rubber	0.104	kg
		0.070	kg
	Low Lead Zinc Oxide	0.044	kg
	Stearic acid	0.009	kg
	MBTS-75	0.004	kg

	WP3	Quantity	Unit
	300 Mesh Sulphur	0.022	kg
	OUTPUT		
	Biorubber panel	**1**	kg
	WASTE		
	Polymer filament	0.108	kg
	EMISSIONS		
	-	-	
	ENERGY REQUIREMENTS		
	Compounding	0.313	kWh/kg
	Compression Moulding	0.283	kWh/kg

In Table 80 the same “Lignin extraction” in 1st scenario and “Rubber functionalization” processes are used for the “current scenario”, but the additive (natural rubber added as acrylonitrile and butadiene) is changed to all rubber as synthetic rubber. The complete substitution to the industrial process is not useful, as mentioned above, because it is complicated and difficult to compare a current industrial scenario with this laboratory scale scenario, so it is an adaptation of the new GREEN-LOOP process, but with the current raw materials.

Table 80. LCI for WP3-current

	WP3	**Quantity**	**Unit**
Lignin extraction 1	**INPUT**		
	Distilled water	35.85	kg
	Sodium sulphide	0.28	kg
	Sodium hydroxide	0.94	kg
	Lignocellulose Biomass	5.56	kg
	Sulfuric Acid 98%	1.10	kg
	OUTPUT		
	Lignin powder	**1**	kg
	WASTE		
	Acid liquor	39.43	kg
	Cellulose rich waste	2.86	kg
	EMISSIONS		
	-		
	ENERGY REQUIREMENTS		
	High-pressure batch reactor	266.54	kWh/kg
Rubber functionalization	**INPUT**		
	Vulcanized rubber crumbs (70% synthetic rubber, 29% carbon black and 1% silica sand)	0.875	kg
		0.3625	kg
		0.0125	kg
	Deep Eutectic Solvent	(+/-) 8.330	kg

	WP3	Quantity	Unit
		(+/-) 16.670	kg
	OUTPUT		
	Devulcanized Rubber (70%)	**1**	kg
	WASTE		
	Waste rubber	2.000	kg
	EMISSIONS		
	-		
	ENERGY REQUIREMENTS		
	Oven 1	14.4	kWh/kg
	Ultrasound equipment	1.32	kWh/kg
	Oven 2	4.8	kWh/kg
Current rubber panel	**INPUT**		
	Devulcanized Rubber (70%)	0.696	kg
	Lignin powder	0.218	kg
	Virgin rubber	0.174	kg
	Low Lead Zinc Oxide	0.0435	kg
	Stearic acid	0.0087	kg
	MBTS-75 (accelerator)	0.00435	kg
	300 Mesh Sulphur	0.0218	kg
	OUTPUT		
	Current Panel	**1**	kg
	WASTE		
	Polymer filament	0.108	kg
	EMISSIONS		
	-	-	
	ENERGY REQUIREMENTS		
	Compounding	0.313	kWh/kg
	Compression Moulding	0.283	kWh/kg

3.2.2.2. Bioplastic manufacture

These tables are showing the inventories for three different scenarios regarding WP4, inside the GREEN-LOOP Project. The structure of the tables is the same as in the previous WP. When entering data in SIMAPRO, the material balance is adjusted in such a way that the output is 1 kg of bio-based material obtained, corresponding to the FU defined above for all value chains.

The Table 81 has the LCI related with the first scenario, wCORK, the production of bio-based closures with a 20% of cork in the formulation. The remaining 80% of the mixture is made up of biodegradable biopolymers, which 70% is poly(3-hydroxybutyrate-co-3-hydroxyhexanoate) (PHBH) and 30% is polylactide acid (PLA).

Table 81. LCI for WP4-wCORK.

	WP4	Quantity	Unit
Olive oil closures (with CORK)	**INPUT**		
	PHBH	0.67	kg
	PLA	0.13	kg
	Cork	0.20	kg
	OUTPUT		
	Bottle closures	1	kg
	WASTE		
	-	-	
	EMISSIONS		
	-	-	
	ENERGY REQUIREMENTS		
	Hopper loader	0.818	kWh/kg
	Extruder	10.95	kWh/kg
	Microwave preheating system	1.095	kWh/kg
	Dehumidifier	0.1044	kWh/kg
	Injection moulding machine	4	kWh/kg

Then, the *Table 82* has the inputs and output related to the 2nd scenario inside the WP4 VC, w/oCORK. In this manufacturing process, the cork is removed from the recipe, so the PHBH is the 70% of the mixture and PLA corresponds to 30%.

Table 82. LCI for WP4-w/oCORK.

	WP4	Quantity	Unit
Olive oil closures (without CORK)	**INPUT**		
	PHBH	0.70	kg
	PLA	0.30	kg
	OUTPUT		
	Bottle closures	1	kg
	WASTE		
	-	-	
	EMISSIONS		
	-	-	
	ENERGY REQUIREMENTS		
	Hopper loader	0.818	kWh/kg
	Extruder	10.95	kWh/kg
	Microwave preheating system	1.095	kWh/kg
	Dehumidifier	0.1044	kWh/kg
	Injection moulding machine	4	kWh/kg

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To take as reference in this value chain, it has been selected the traditional materials for olive oil closures [34] as the “current scenario”. As in the previous case, the energy consumption will be the same for all scenarios for an equivalent production scale. All this information is represented in Table 83.

Table 83. LCI for WP4-current.

	WP4	Quantity	Unit
Current Plastic closures	**INPUT**		
	Aluminium	0.50	kg
	LDPE	0.50	kg
	OUTPUT		
	Bottle closures	1	kg
	WASTE		
	-	-	
	EMISSIONS		
	-	-	
	ENERGY REQUIREMENTS		
	Hopper loader	0.818	kWh/kg
	Extruder	10.95	kWh/kg
	Microwave preheating system	1.095	kWh/kg
	Dehumidifier	0.1044	kWh/kg
	Injection moulding machine	4	kWh/kg

3.2.2.3. Wood composite manufacture

In WP5, several compositions of the wood composite mix have been tested and all of them have been analysed from the environmental perspective. In this report, two different mixes will be selected to show their results in detail and to be compared with the current scenario as a reference case.

As it was mentioned above, only MIX1 and MIX3 were selected for these analyses due to these both mixtures are the most environmentally favourable and the worst one, as it is showed in Figure 61 (this Figure will be commented in next chapter). All inventory data have been collected for all mixtures, but as the analysis will only be carried out for mixtures 1 and 3, only these have been added. The inventory for the wood composites manufacturing with MIX1 is shown in *Table 84*, with a 50-50% of wood and biopolymer. The Offcuts of this MIX1 are considered with the same composition as the raw materials defined in the inputs of the system. The FU selected is the manufacturing of 1 kg of wood composite produced.

Table 84. LCI for WP5-MIX1.

	WP5	Quantity	Unit
Wood composites production (MIX1)	**INPUT**		
	Bio-Polymer	0.6785	kg
	Wood	0.6785	kg
	OUTPUT		
	Wood composite	1	kg

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	WP5	Quantity	Unit
	WASTE		
	Offcuts WC1	0.158	kg
		0.158	kg
	EMISSIONS		
	-	-	
	ENERGY REQUIREMENTS		
	Eirich Mixer	4.05	kWh/kg
	Microwaves	5.25	kWh/kg
	Extruder	0.75	kWh/kg
	Kneader machine	0.37	kWh/kg
	Compression moulding	13.6	kWh/kg
	Machining	24	kWh/kg

The inventory for the second scenario analysed in this WP4, MIX3, is collected in *Table 85*.The ratio of the mixture is different from the previous MIX1. The MIX3 has the following percentages in its composition: 59.4% of biopolymer, 39.6% of wood, and 1% of graphite. As in the previous scenario, the offcuts have the same structure as the inputs, and the energy requirements are the same.

Table 85. LCI for WP5-MIX3.

	WP5	Quantity	Unit
Wood composites production (MIX3)	**INPUT**		
	Bio-Polymer	0.94268	kg
	Wood	0.62845	kg
	Graphite	0.01587	kg
	OUTPUT		
	Wood composite	1	kg
	WASTE		
	Offcuts WC3	0.34868	kg
		0.23245	kg
		0.00587	kg
	EMISSIONS		
	-	-	
	ENERGY REQUIREMENTS		
	Eirich Mixer	4.05	kWh/kg
	Microwaves	5.25	kWh/kg
	Extruder	0.75	kWh/kg
	Kneader machine	0.37	kWh/kg
	Compression moulding	13.6	kWh/kg
	Machining	24	kWh/kg

A very common material [35]for sliding bearings is the bronze and copper alloys, so this will be the reference system as “current” production. The offcuts will be scraps from the metallic material, and as in the previous WPs, the energy requirements will be the same due to the difficult comparison between the scales. The FU is 1 kg of metallic component produced. The inventory for this current material is collected in *Table 86*.

Table 86. LCI for WP5-current

	WP5	Quantity	Unit
Metallic composites production	**INPUT**		
	Copper alloy	1.587	kg
	OUTPUT		
	Metal composite	1	kg
	WASTE		
	Offcuts (scraps)	0.587	kg
	EMISSIONS		
	-	-	
	ENERGY REQUIREMENTS		
	Eirich Mixer	4.05	kWh/kg
	Microwaves	5.25	kWh/kg
	Extruder	0.75	kWh/kg
	Kneader machine	0.37	kWh/kg
	Compression moulding	13.6	kWh/kg
	Machining	24	kWh/kg

4. Analysis of results

4.1. Energy analysis

4.1.1. Bio-rubber manufacture

Lignin extraction

Table 87. Energy contributions for each of the steps in lignin extraction process.

Process unit	Pulping	Filtration 1	Acidification	Filtration 2	Washing	Drying
$(\dot{m}_k \cdot h_k)_{in}$ [kJ]	0	493.85	0	0	0	0
$(\dot{m}_k \cdot h_k)_{out}$ [kJ]	493.85	239.75	0	0	0	83.47
$\dot{Q}_{int}$ [kJ]	-33288	-257.16	-3.06	-3.06	0	83.47
$\dot{W}_{shaft}$ [kJ]	33782	3.06	3.06	3.06	0	0
$\sum \Delta H_R^{Tref}$ [kJ]	Unknown	0	0	0	0	0

Pulping

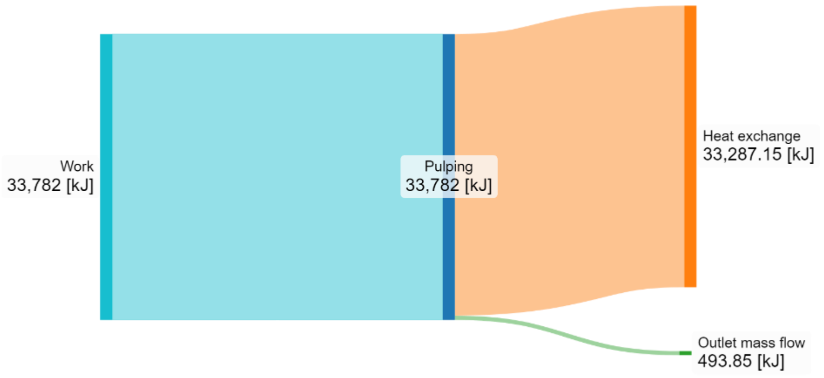

Figure 19. Sankey diagram of energy in pulping step of lignin extraction process.

Work energy required during pulping process is considerably higher than the energy required in the rest of the steps of the process, since the process takes place in a reactor, a device that consume a huge amount of energy. During the process, the separation of lignocellulosic biomass into cellulose, hemicellulose and lignin occurs, but it is not possible to quantify the energy removed or released during that reaction, as there is not data available in literature. The enthalpy of the reaction is extremely dependent on the conditions of the process, such as temperature, pressure, the proportion of the different components in the biomass, among others. Therefore, to obtain a good estimation, the enthalpy should be measured experimentally. The lack of data implies that the heat exchange is not well quantified. The reaction is endothermic, which would mean that heat exchange should be smaller.

Filtration 1

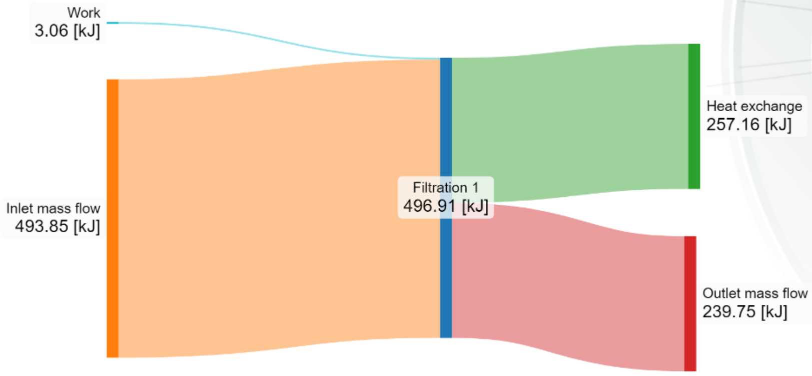

Figure 20. Sankey diagram of energy in first filtration step of lignin extraction process.

This first filtration step does not require a huge amount of work energy, as it takes place using a Büchner funnel, a laboratory equipment that do not involve great amounts of energy. Due to the differences in temperature in the inlet and outlet mass flows, there is a significant amount of heat released.

Acidification

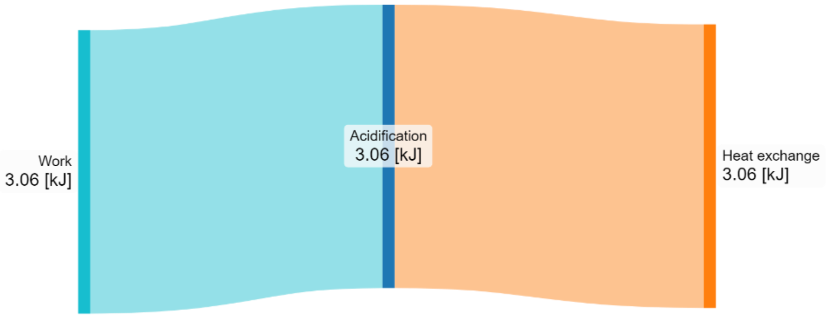

Figure 21. Sankey diagram of energy in acidification step of lignin extraction process.

In this step, only a magnetic stirrer is used to mix the solution, which an equipment used daily in laboratory, which does not require great amounts of energy.

Filtration 2

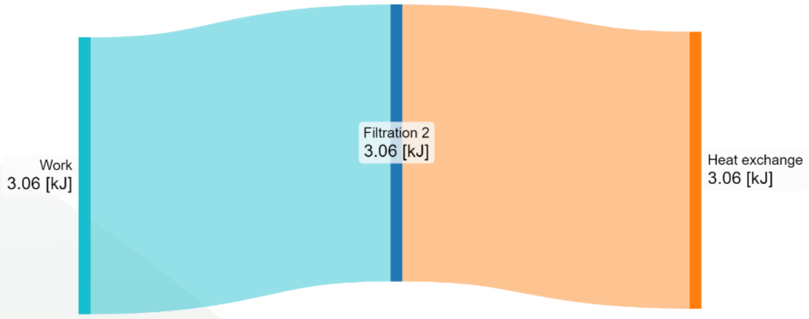

Figure 22. Sankey diagram of energy in second filtration step of lignin extraction process.

In this second filtration, the same as in acidification occur, but in this case using a Büchner funnel.

Washing

Washing is done manually, which means that no work is required, and as there are no changes in temperature, there is not nay heat exchange.

Drying

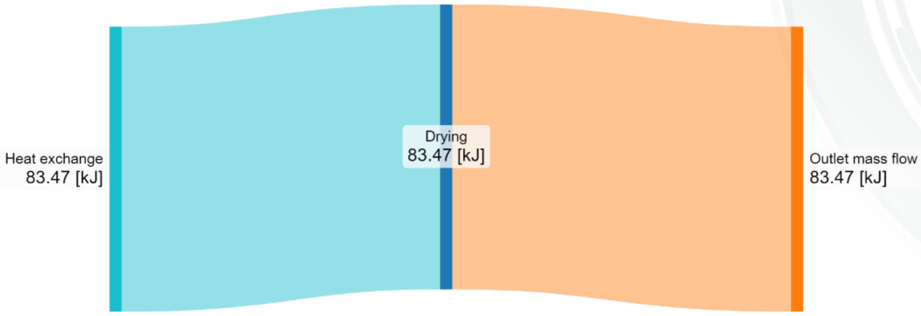

Figure 23. Sankey diagram of energy in drying step of lignin extraction process.

The drying process requires energy to heat the samples and evaporates the remaining liquid, which means that heat exchange is positive in this case.

Rubber functionalisation

Table 88. Energy contributions for each of the steps in rubber functionalisation process.

Process unit	Sonication	Heating	Filtration
$(\dot{m}_k \cdot h_k)_{in}$ [kJ]	0	0	701.07
$(\dot{m}_k \cdot h_k)_{out}$ [kJ]	0	701.07	0
$\dot{Q}_{int}$ [kJ]	-100.98	701.07	-707.19
$\dot{W}_{shaft}$ [kJ]	100.98	0	6.12
$\sum \Delta H_R^{Tref}$ [kJ]	0	0	0

Sonication

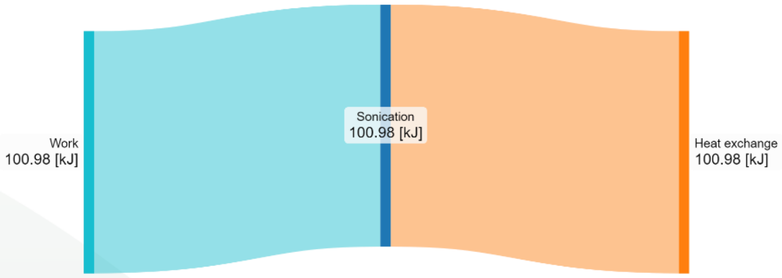

Figure 24. Sankey diagram of energy in sonication step of rubber functionalisation process.

During sonication, mechanical energy in the form of work is used to mix the components, and as a consequence heat is released.

Heating

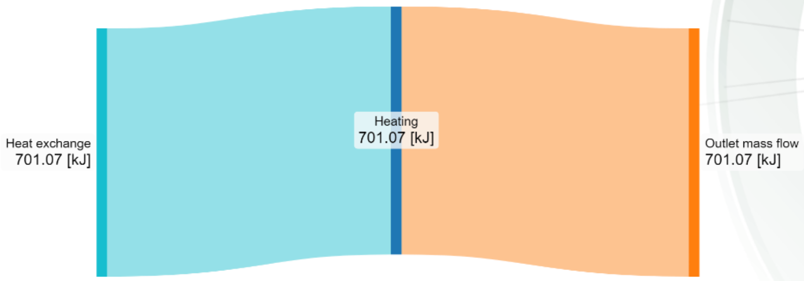

Figure 25. Sankey diagram of energy in heating step of rubber functionalisation process.

During the heating process energy is required to heat the different components. In this case, a deep eutectic solvent huge is heated, which is characterized as being non-volatile. Therefore, there are not phase changes. A high quantity of materials is heated, which implies a considerable amount of energy requirements.

Filtration

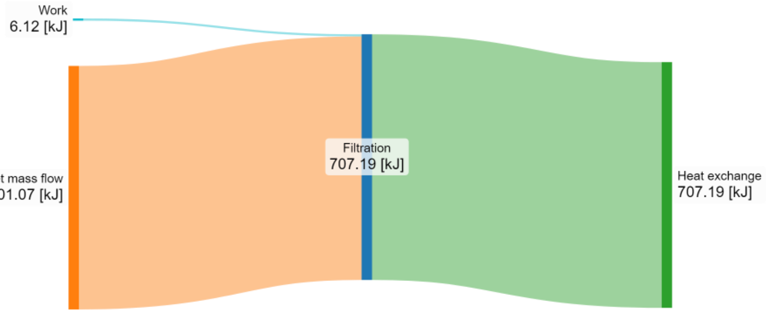

Figure 26. Sankey diagram of energy in filtration step of rubber functionalisation process.

In filtration step, energy derived from work is low compared to the step that requires more energy in this process, which is sonication. Filtration is done with a filter that do not consume great amounts of energy. A huge amount of heat is released because the samples were heated in the previous step, and during filtration the samples reaches ambient temperature.

Rubber panel production

Table 89. Energy contributions for each of the steps in rubber panel production process.

Process unit	Compounding	Cooling	Cutting	Compression moulding	Machining
$(\dot{m}_k \cdot h_k)_{in}$ [kJ]	0	2.18	0	0	0
$(\dot{m}_k \cdot h_k)_{out}$ [kJ]	2.29	0	0	0	0
$\dot{Q}_{int}$ [kJ]	-109.77	-2.18	0	-433	0
$\dot{W}_{shaft}$ [kJ]	112.06	0	0	433	0
$\sum \Delta H_R^{Tref}$ [kJ]	0	0	0	0	0

Compounding

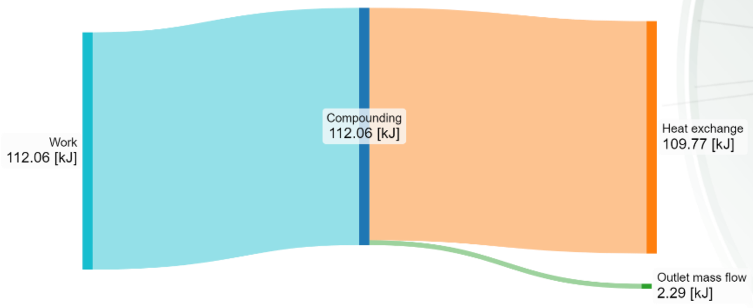

Figure 27. Sankey diagram of energy in compounding step of rubber panel production process.

During compounding, the samples are slightly heated to 40 °C, which implies a smaller increase in the energy derived from outlet mass flows. The work done by the mixer involve losses as heat released.

Cooling

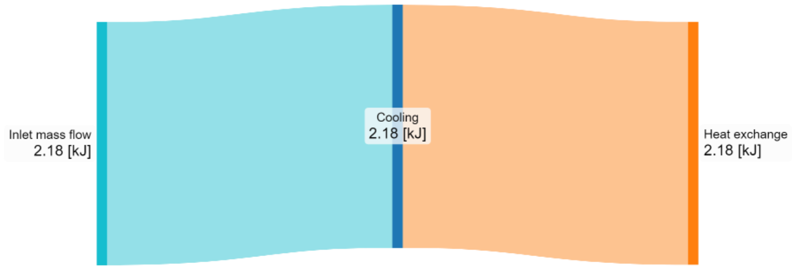

Figure 28. Sankey diagram of energy in cooling step of rubber panel production process.

Cooling is done at ambient temperature, and the samples that were heated previously at 40 °C, reaches ambient temperature.

Cutting

The cutting step is done manually, so there is not work contribution. The samples are not heated or cooled, which means that there is not heat exchange either.

Compression moulding

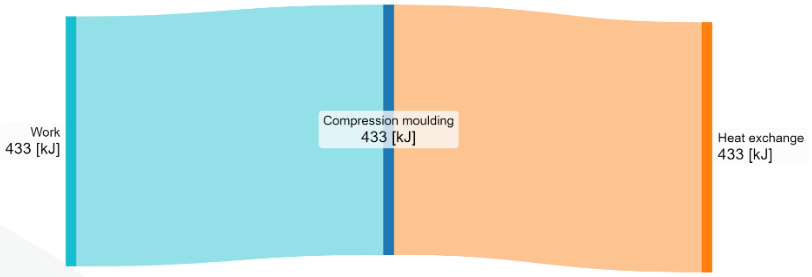

Figure 29. Sankey diagram of energy in compression moulding step of rubber panel production process.

The compression moulding step involves the utilisation of a press, an equipment that requires great amounts of energy. Losses are released as heat.

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Machining

As the cutting step, machining is done manually, so there is not work contribution. The samples are not heated or cooled, which means that there is not heat exchange either.

4.1.2. Bioplastic manufacture

Table 90. Energy contributions for each of the steps in bioplastic manufacture process.

Process unit	Dispensation	Extrusion	Injection moulding
$(\dot{m}_k \cdot h_k)_{in}$ [kJ]	476.4	476.4	2259.1
$(\dot{m}_k \cdot h_k)_{out}$ [kJ]	476.4	2259.1	0
$\dot{Q}_{int}$ [kJ]	0	-333287	-124659.1
$\dot{W}_{shaft}$ [kJ]	0	335070	122400
$\sum \Delta H_R^{Tref}$ [kJ]	0	0	0

Dispensation

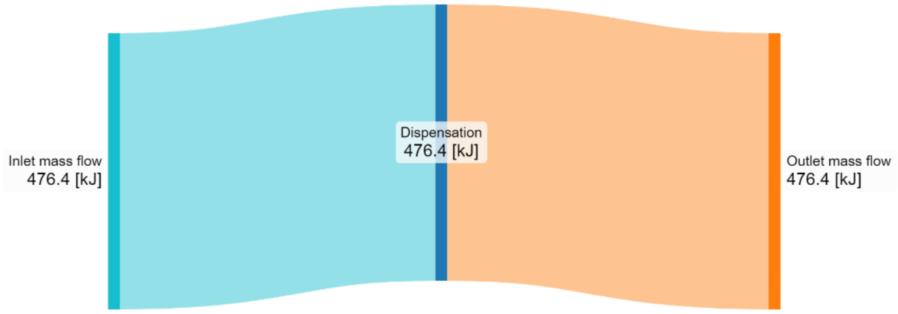

Figure 30. Sankey diagram of energy in dispensation step of bioplastic production process.

Materials are previously heated before introducing them in the hopper, and they leave it at the same temperature. Therefore, there is not heat exchange. As the process is done manually, there is not work involved.

Extrusion

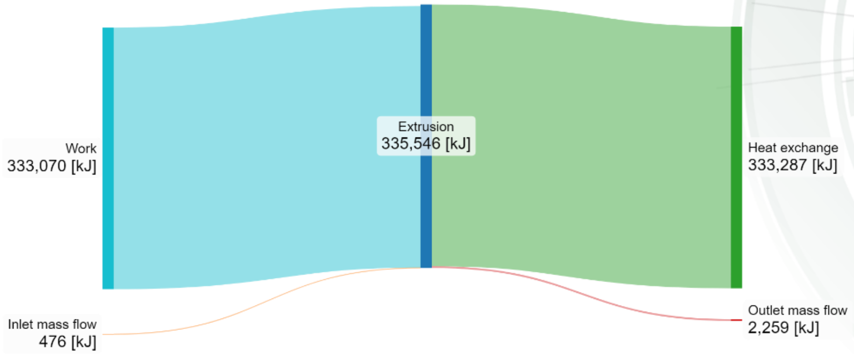

Figure 31. Sankey diagram of energy in extrusion step of bioplastic production process.

In this step, an extrusion equipment is utilised to process the materials. An extruder is a device that exert huge amounts of energy to the processed materials, which explain why work term is as remarkable. Even though, the values obtained should not be that big. The data used to calculate the energy contributions was extracted from LCI templates but doubts about its validity arises.

Injection moulding

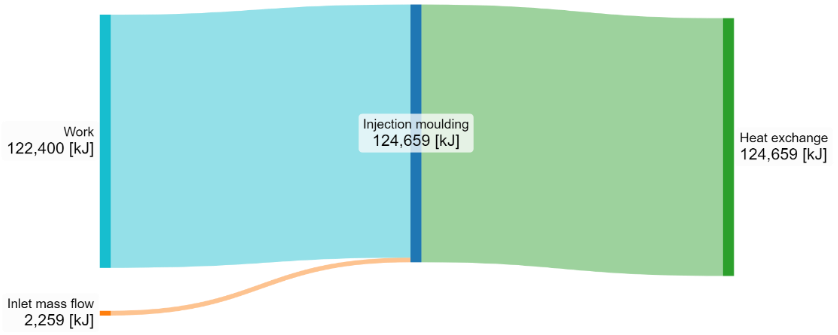

Figure 32. Sankey diagram of energy in injection moulding step of bioplastic production process.

In injection moulding step, the same problem that in the previous step arises. Data was obtained in LCI template rather than the templates. Work value should also be high, but not as high as the result obtained. In bibliography *[36]*, it was found that an extrusion process (considering both extrusion and moulding) has an energy consumption of 2.5 kWh/kg as maximum. In this case, the total energy consumption of injection moulding and extrusion is around 15 kWh/kg, six times the maximum expected consumption.

4.1.3. Wood composites manufacture

Table 91. Energy contributions for each of the steps in wood composite manufacture process.

Process unit	Mixing	Extrusion	Kneading	Compression moulding	Machining
$(\dot{m}_k \cdot h_k)_{in}$ [kJ]	0	377.28	377.28	0	345.84
$(\dot{m}_k \cdot h_k)_{out}$ [kJ]	377.28	377.28	0	377.28	0
$\dot{Q}_{int}$ [kJ]	-7272.72	-6885	-3734.28	-20124.72	-345.84

Process unit	Mixing	Extrusion	Kneading	Compression moulding	Machining
$\dot{W}_{shaft}$ [kJ]	7650	6885	3366	20502	0
$\sum \Delta H_R^{Tref}$ [kJ]	0	0	0	0	0

Mixing

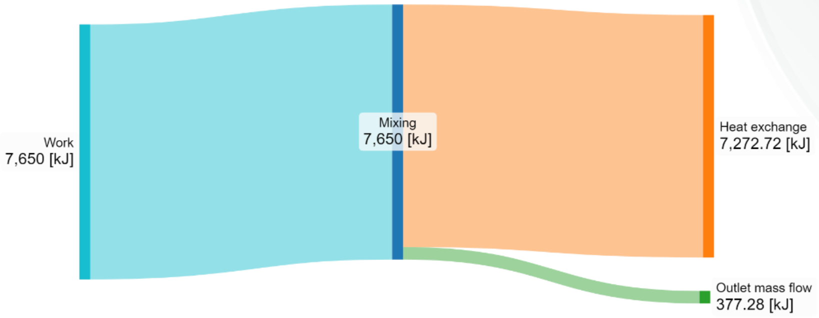

Figure 33. Sankey diagram of energy in mixing step of wood composite production process.

During this step, samples are mixed and heated. Heat exchange represents the sum of the heat provided by the heating device and the heat losses produced during the process.

Extrusion

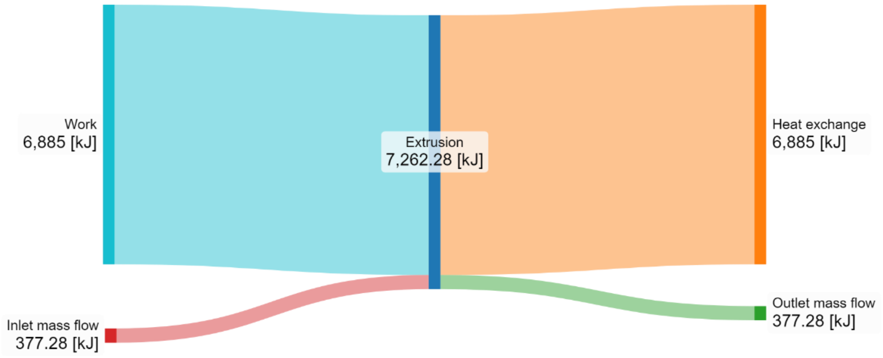

Figure 34. Sankey diagram of energy in extrusion step of wood composite production process.

During extrusion, the samples leave the equipment at the same temperature that they enter, because a microwave device is used to maintain it. Heat exchange includes again the heat losses and the heat generated by the microwave device.

Kneading

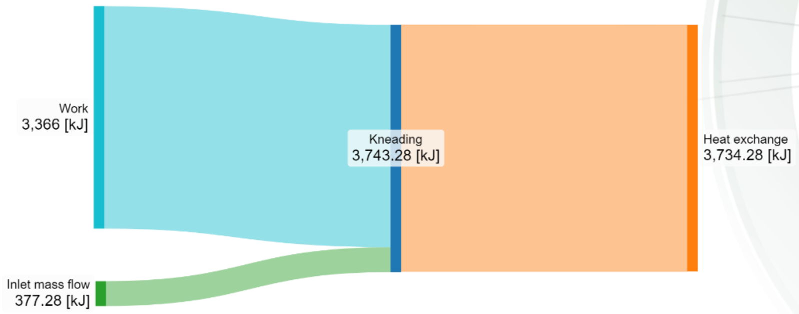

Figure 35. Sankey diagram of energy in kneading step of wood composite production process.

During this step, the samples are cooled until room temperature, as no heat device is used.

Compression moulding

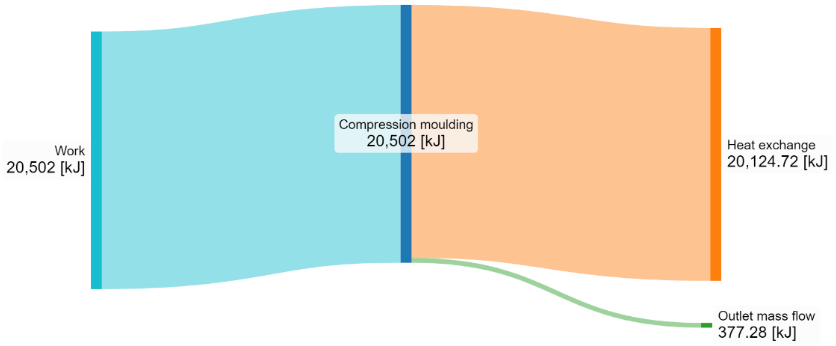

Figure 36. Sankey diagram of energy in compression moulding step of wood composite production process.

In compression moulding, the samples are heated. A remarkable amount of work is involved in the process, as press machines requires a lot of energy.

Machining

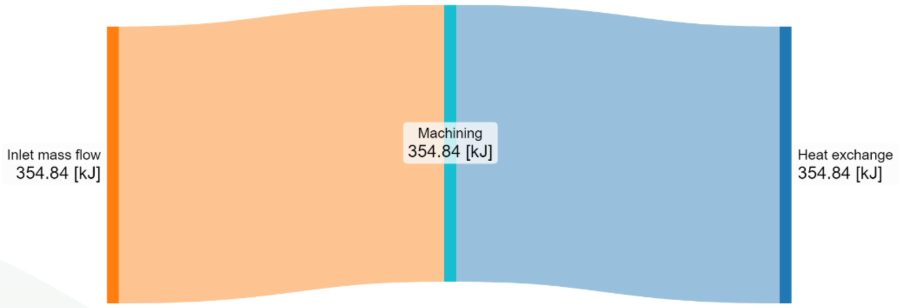

Figure 37. Sankey diagram of energy in machining step of wood composite production process.

During machining, work energy is dissipated in the form of heat.

4.2. Exergy analysis

4.2.1. Bio rubber manufacture

Lignin extraction

Table 92. Exergy contributions for each of the steps in lignin extraction process.

Process unit	Pulping	Filtration 1	Acidification	Filtration 2	Washing	Drying
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	0	93.85	0	0	0	0
$(\mathrm{m}_k \cdot \psi)_{out}$ [kJ]	93.85	45.56	0	0	0	1.44
$\left(1-\frac{T_0}{T_k}\right)Q_{int}$ [kJ]	-11145	0	0	0	0	16.78
W [kJ]	33782	3.06	3.06	3.06	0	0
$T_0 S_{gen}$ [kJ]	22543.15	51.35	3.06	3.06	0	15.34

Pulping

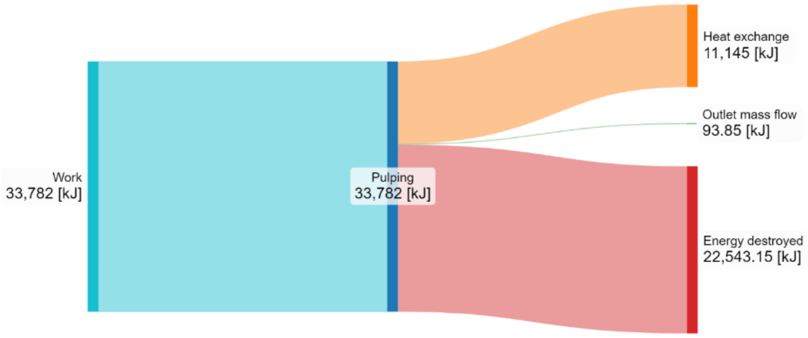

Figure 38. Sankey diagram of exergy in pulping step of lignin extraction process.

In pulping step, the energy destroyed (also called irreversibility) is considerably high, as the reactor in which the process takes place requires energy that is dissipated in the form of heat that cannot be used. Note that the results for this step are not fully accurate, as the heat exchange should be different. The energy required in the reactions that occur in the reactor is not quantified, as explained in energy analysis section.

Filtration 1

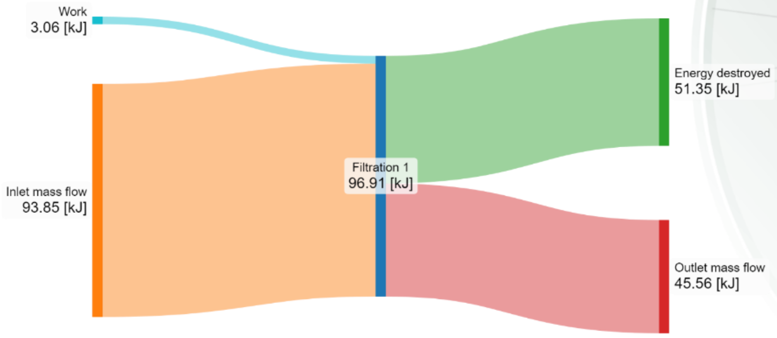

Figure 39. Sankey diagram of exergy in first filtration step of lignin extraction process.

In this step, part of the energy is lost, and other part leaves the system in the outlet mass.

Acidification

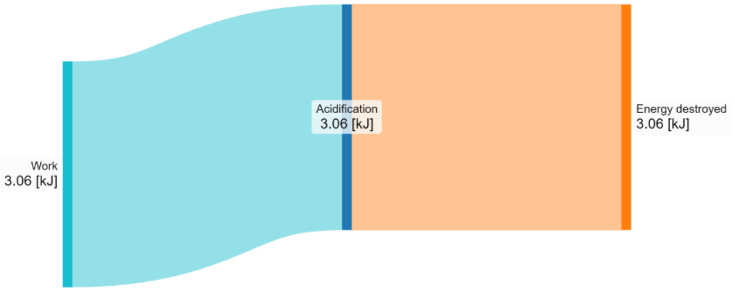

Figure 40. Sankey diagram of exergy in acidification step of lignin extraction process.

The work used during this step is lost during the process.

Filtration 2

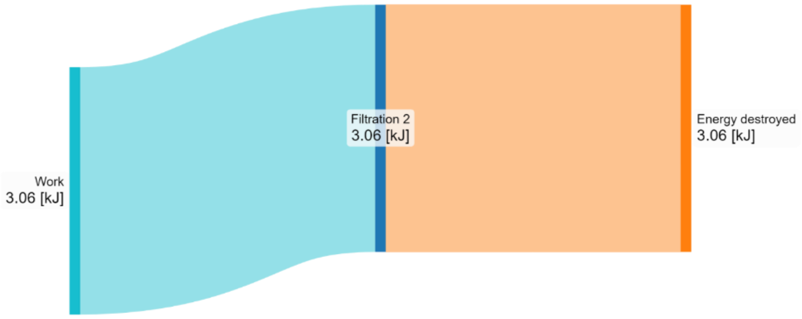

Figure 41. Sankey diagram of exergy in second filtration step of lignin extraction process.

As in acidification step, the work used during this step is lost during the process.

Washing

In washing step there is not any form of energy involved.

Drying

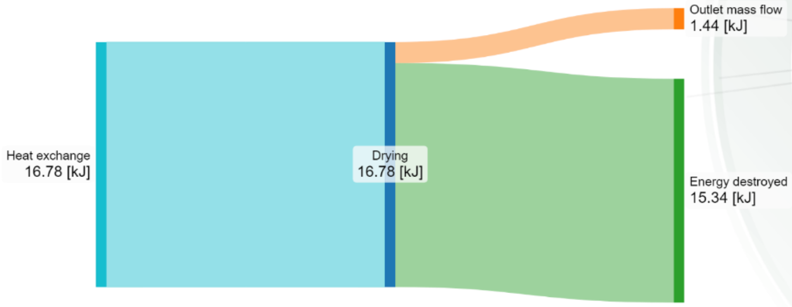

Figure 42. Sankey diagram of exergy in drying step of lignin extraction process.

Most of the heat employed in drying step is lost, and a small portion of it is employed in drying the samples.

Rubber functionalisation

Table 93. Exergy contributions for each of the steps in rubber functionalisation process.

Process unit	Sonication	Heating	Filtration
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	0	0	136.59
$(\mathrm{m}_k \cdot \psi)_{out}$ [kJ]	0	136.59	0
$\left(1-\frac{T_0}{T_k}\right) Q_{int}$ [kJ]	0	239.88	0
W [kJ]	100.98	0	6.12
$T_0 S_{gen}$ [kJ]	100.98	103.29	142.71

Sonication

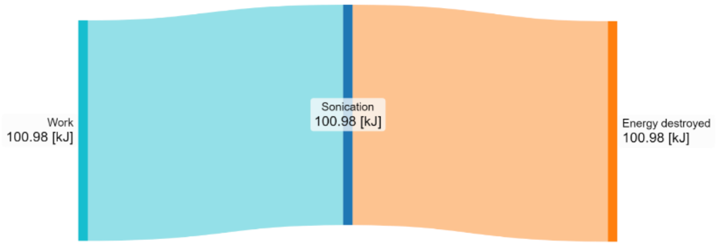

Figure 43. Sankey diagram of exergy in sonication step of rubber functionalisation process.

All the energy derived from work in this step is lost along the process.

Heating

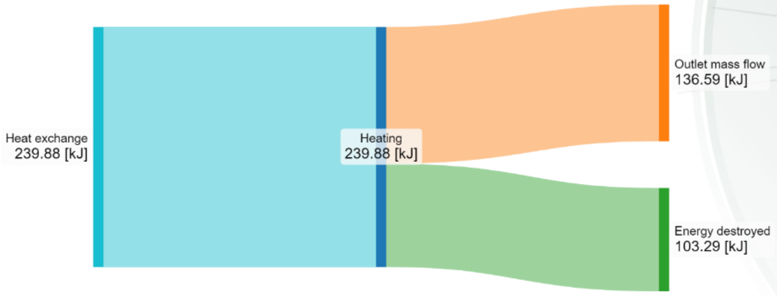

Figure 44. Sankey diagram of exergy in heating step of rubber functionalisation process.

During the heating process, a part of the energy heats the samples and another part is lost.

Filtration

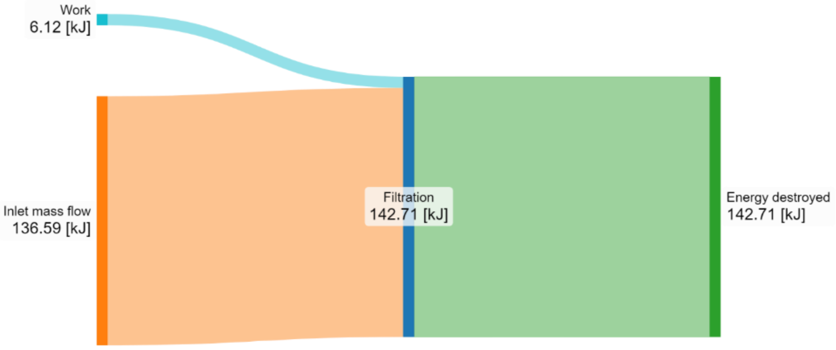

Figure 45. Sankey diagram of exergy in filtration step of rubber functionalisation process.

During the filtration step, all the energy is destroyed during the process.

Rubber panel production

Table 94. Exergy contributions for each of the steps in rubber panel production process.

Process unit	Compounding	Cooling	Cutting	Compression moulding	Machining
$(m_k \cdot \psi)_{in}$ [kJ]	0	0.053	0	0	0
$(m_k \cdot \psi)_{out}$ [kJ]	0.055	0	0	0	0
$\left(1-\frac{T_0}{T_k}\right) Q_{int}$ [kJ]	-5.26	0	0	-135	0
W [kJ]	112.06	0	0	433	0
$T_0 S_{gen}$ [kJ]	106.75	0.053	0	298	0

Compounding

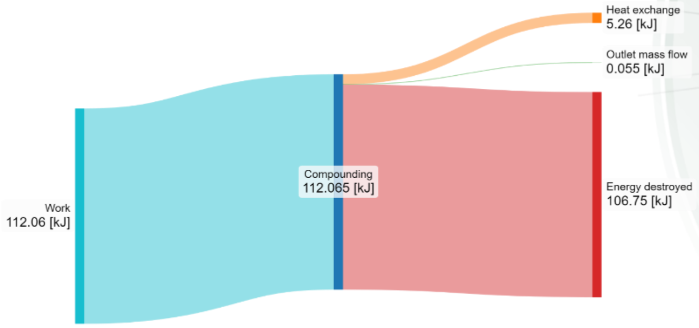

Figure 46. Sankey diagram of exergy in compounding step of rubber panel production process.

In compounding step, most of the energy used is lost during the process. A small portion is used to heat the samples, as the samples are only heated at 40 °C.

Cooling

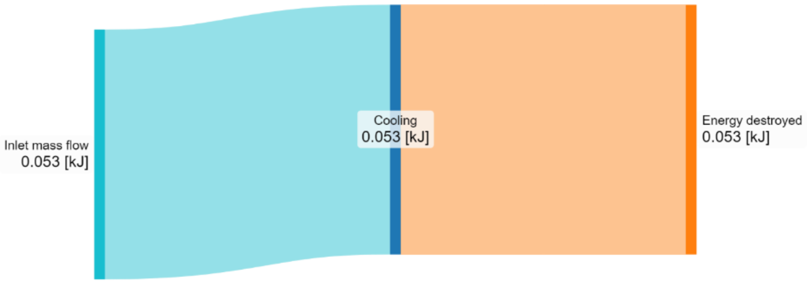

Figure 47. Sankey diagram of exergy in cooling step of rubber panel production process.

Cooling is done at ambient temperature, and therefore all the energy is lost.

Cutting

In cutting step there are not any form of energy involved.

Compression moulding

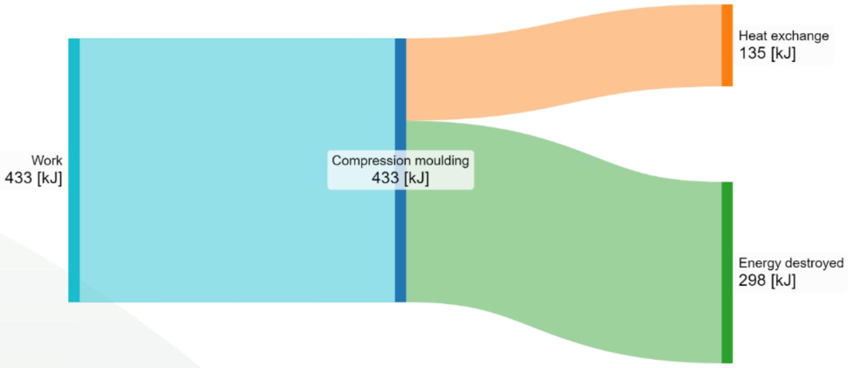

Figure 48. Sankey diagram of exergy in compression moulding step of rubber panel production process.

In compression moulding step, a significant portion of energy is lost, and the rest is dissipated in the form of heat.

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Machining

In machining step there are not any form of energy involved.

4.2.2. Bioplastic manufacture

Table 95. Exergy contributions for each of the steps in bioplastic manufacture process.

Process unit	Dispensation	Extrusion	Injection moulding
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	22.06	22.06	418.32
$(\mathrm{m}_k \cdot \psi)_{out}$ [kJ]	22.06	418.32	0
$\left(1-\frac{T_0}{T_k}\right) Q_{int}$ [kJ]	0	-109089	0
W [kJ]	0	335070	122400
$T_0 S_{gen}$ [kJ]	0	225584	122818.32

Dispensation

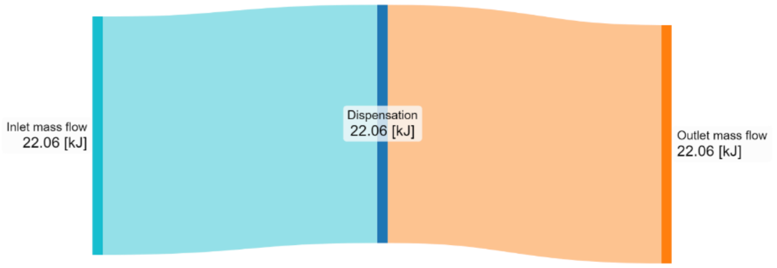

Figure 49. Sankey diagram of exergy in dispensation step of bioplastic production process.

During this step there is no energy destroyed, as the components enter and leave the system at the same temperature. Also, the process is done manually, and there is not work involved.

Extrusion

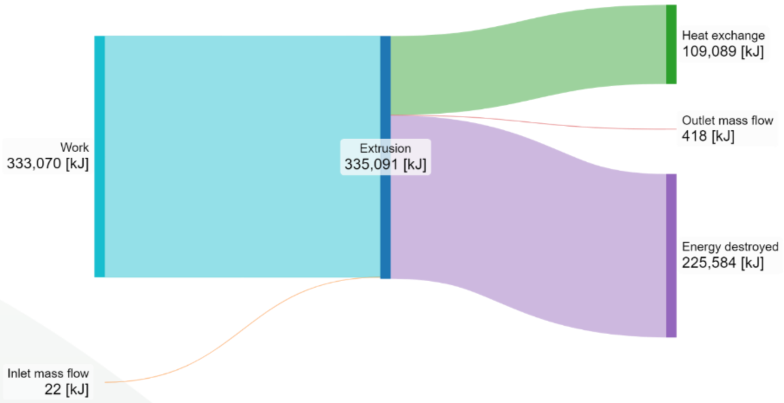

Figure 50. Sankey diagram of exergy in extrusion step of bioplastic production process.

Most of the energy generated in the system becomes useless. A smaller portion is dissipated in the form of energy. Note that, as explained in energy analysis section, the data is not fully accurate.

Injection moulding

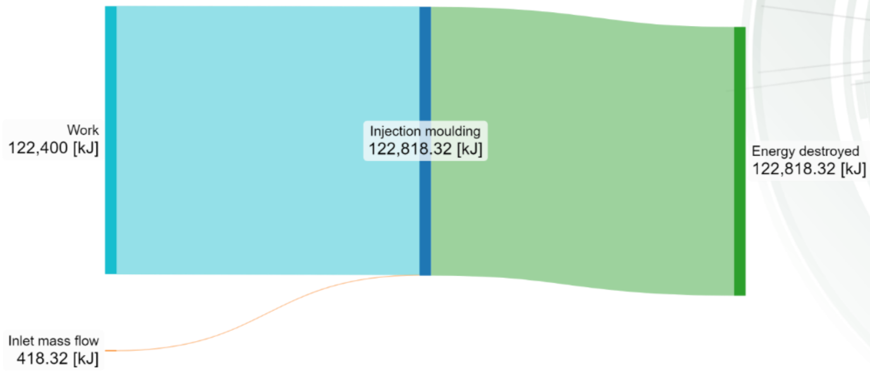

Figure 51. Sankey diagram of exergy in injection moulding step of bioplastic production process.

All the energy derived from work in this step is lost along the process. As explained in energy analysis section, the results obtained are not fully accurate.

4.2.3. Wood composites manufacture

Table 96. Exergy contributions for each of the steps in wood composite manufacture process.

Process unit	Mixing	Extrusion	Kneading	Compression moulding	Machining
$(\mathrm{m}_k \cdot \psi)_{in}$ [kJ]	0	80.47	80.47	0	73.76
$(\mathrm{m}_k \cdot \psi)_{out}$ [kJ]	80.47	80.47	0	80.47	0
$\left(1-\frac{T_0}{T_k}\right) Q_{int}$ [kJ]	-2690.75	-2547.30	0	-7445.72	0
W [kJ]	7650	6885	3366	20502	0
$T_0 S_{gen}$ [kJ]	4878.48	4337.70	3446.47	12975.81	73.76

Mixing

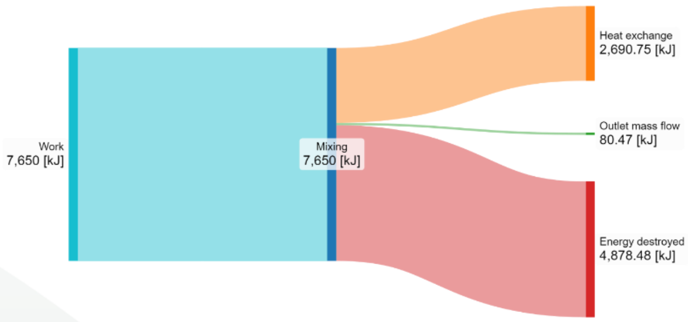

Figure 52. Sankey diagram of exergy in mixing step of wood composite production process.

Most of the energy generated during mixing step is lost, and a part of it is dissipated as heat. In this case, the energy destroyed is considerable, as the process demands a huge amount of work.

Extrusion

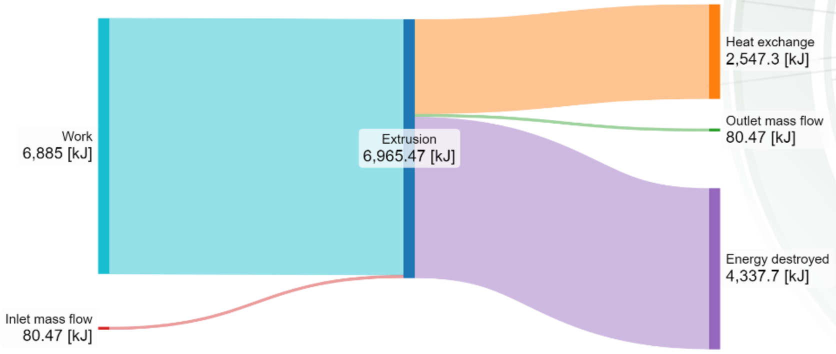

Figure 53. Sankey diagram of exergy in extrusion step of wood composite production process.

Most of the energy generated during extrusion is lost, and a small portion is dissipated as heat. As in the previous step, a huge amount of energy is lost because the process involves a great use of energy.

Kneading

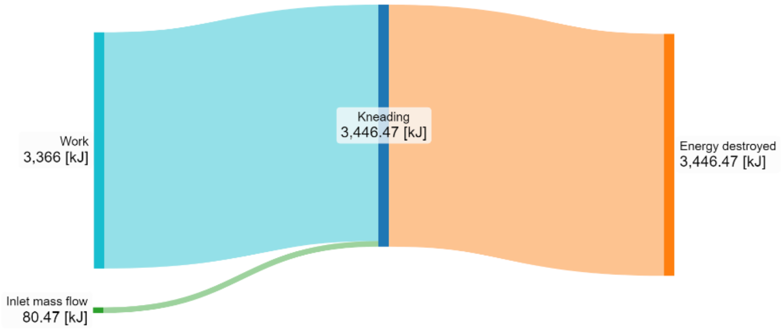

Figure 54. Sankey diagram of exergy in kneading step of wood composite production process.

All the energy derived from work in this step is lost along the process.

Compression moulding

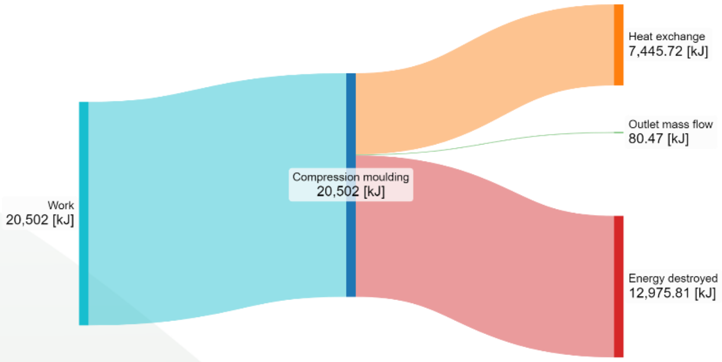

Figure 55. Sankey diagram of exergy in compression moulding step of wood composite production process.

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Most of the energy generated during compression moulding is lost, and a small portion is dissipated as heat. The heat dissipated could be used if necessary.

Machining

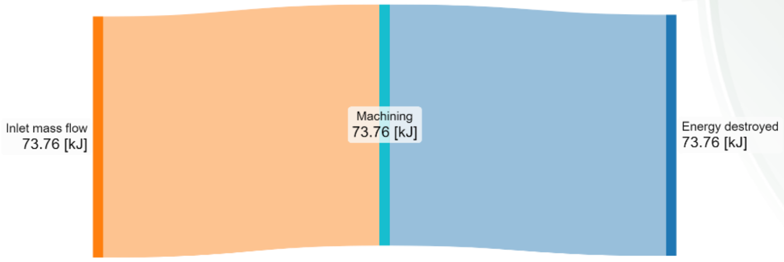

Figure 56. Sankey diagram of exergy in machining step of wood composite production process.

The samples enter the system at a high temperature, and all that energy is lost during the step. There is no work in the process as the process is done manually.

4.3. LCA results

4.3.1. Bio-rubber manufacture

It was analysed the impact of each of the steps of the process and the contribution of different categories (raw materials, electricity and waste). In Figure 57, the contribution of each category to the impact is presented. For all the scenarios analysed the main contribution (in mPt) is 'Ionizing radiation HH', represented in light green; followed by 'Mineral, fossil & ren resource depletion', the yellow on top. In this Figure, it is possible to see that when the bio-rubber panel is obtained by the GREEN-LOOP Process with bio-based material than the same process but with virgin petroleum-based material. All the data and results for WP3 process shown in Figure 57**Error! Reference source not found.** are collected in Environmental impact categories for WP3.Table 97, divided by environmental impact categories.

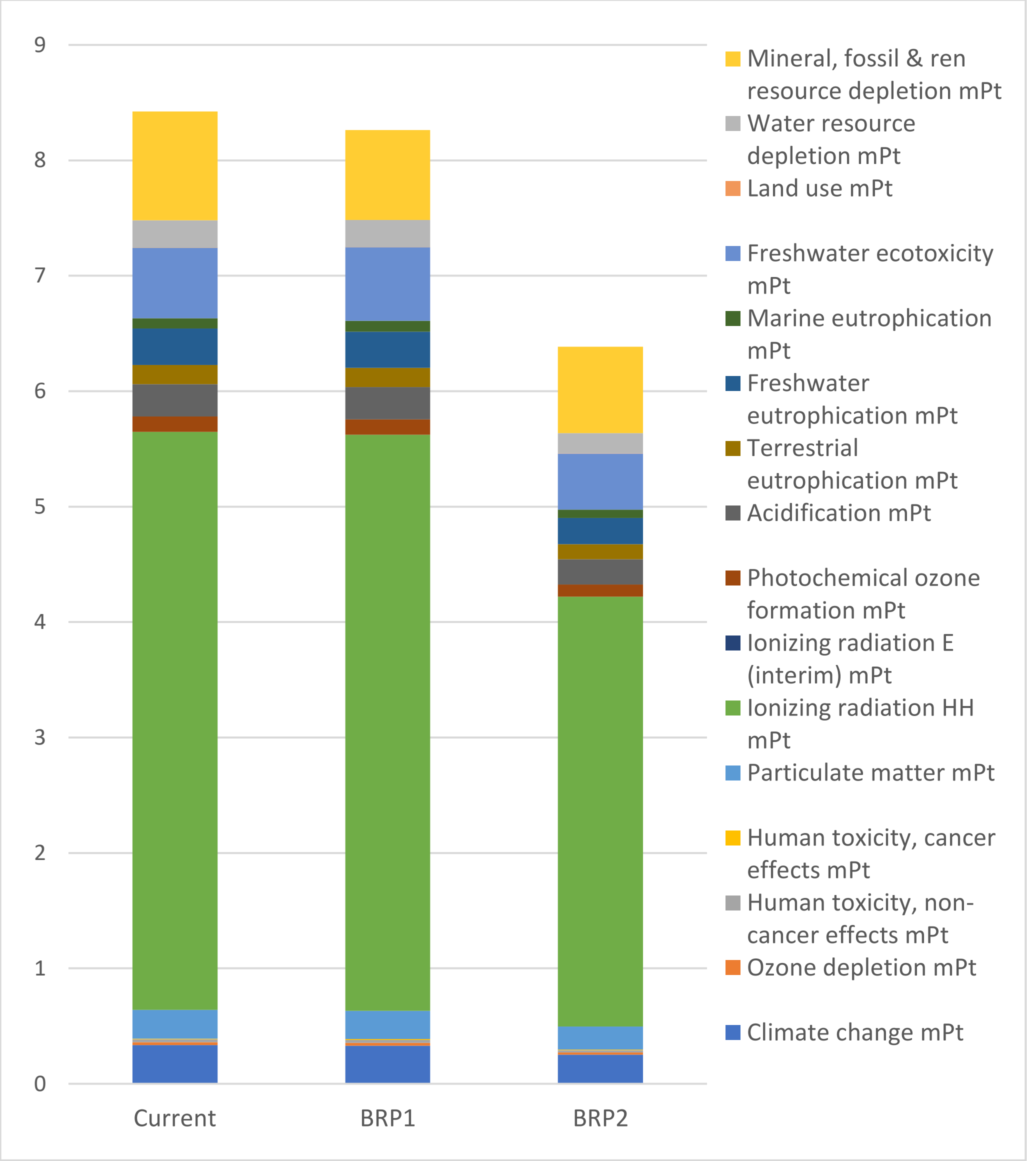

Figure 57. Environmental impacts categories (mPt) of WP3 scenarios.

The main environmental contribution for environmental impact in all scenarios is the electricity consumption in the manufacturing process, as it represented in Figure 58. However, it is important to note that when using the small reactor and the ultrasound sonicator, the electricity consumption decreases compared to the larger reactor. Another interesting remark is that the environmental impacts of Raw Materials is higher with the synthetic rubber than with natural rubber.

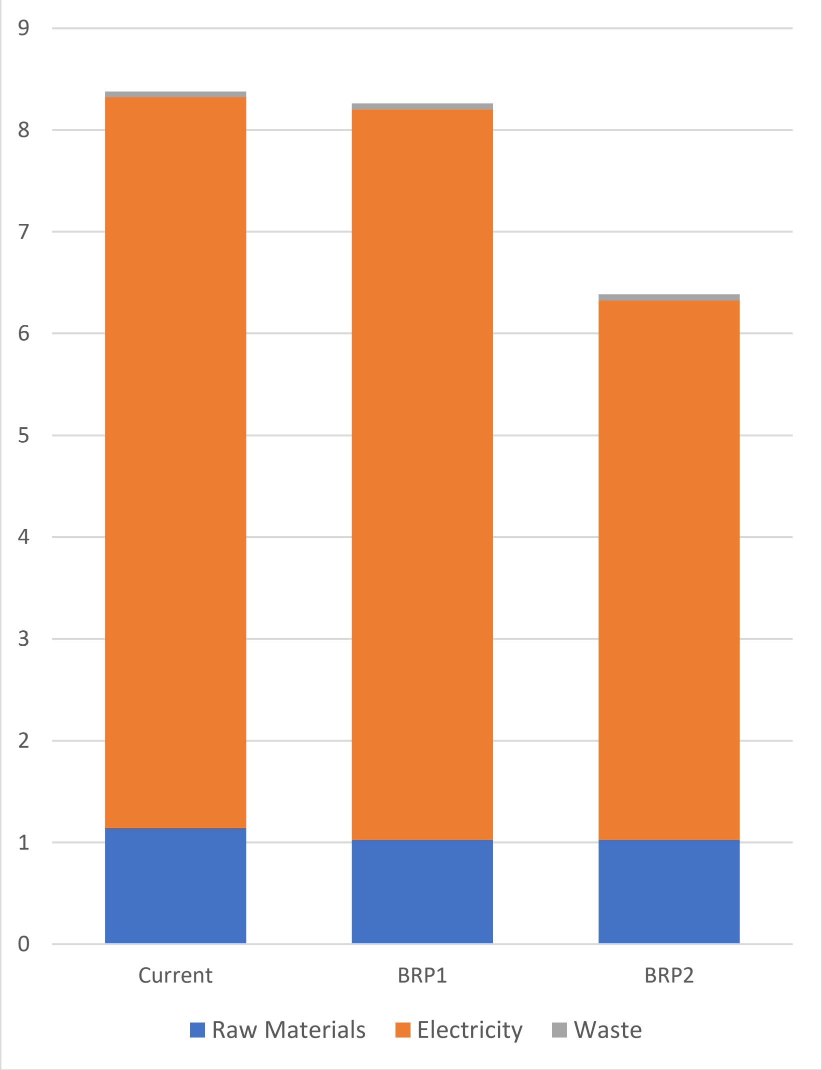

Figure 58. Environmental impacts by Process contribution (mPt) of WP3 scenarios.

As it is possible to see in Table 97, it is important to highlight some several decreases generated during the application of the GREEN-LOOP Project systems. The BRP1 case has decreased the *Mineral, fossil & ren resource depletion* impact a 18%, while the BRP2 has decreased the *Ionizing radiation HH* impact a 26% with the current situation as reference in both cases.

Table 97. Environmental impact categories for WP3.

Impact categories	Unit	Current	BRP1	BRP2
Climate change	mPt	0.335	0.330	0.253
Ozone depletion	mPt	0.0254	0.0250	0.0198
Human toxicity, non-cancer effects	mPt	0.0245	0.0256	0.0197
Human toxicity, cancer effects	mPt	0.00549	0.00573	0.00477
Particulate matter	mPt	0.249	0.247	0.199
Ionizing radiation HH	mPt	5.006	4.990	3.724
Ionizing radiation E (interim)	mPt	0	0	0
Photochemical ozone formation	mPt	0.133	0.132	0.105
Acidification	mPt	0.281	0.281	0.220
Terrestrial eutrophication	mPt	0.166	0.167	0.131
Freshwater eutrophication	mPt	0.316	0.315	0.226
Marine eutrophication	mPt	0.0892	0.0918	0.0733
Freshwater ecotoxicity	mPt	0.610	0.638	0.485
Land use	mPt	0.000616	0.000600	0.000508
Water resource depletion	mPt	0.238	0.237	0.177
Mineral, fossil & ren resource depletion	mPt	0.945	0.777	0.747

4.3.2. Bioplastic manufacture

In Figure 59 it is possible to review the contribution of each category. The main contribution is the Ionizing radiation HH, followed by Freshwater ecotoxicity. Comparing the three scenarios with each other, the current situation has the highest sum of impacts than the other two scenarios from GREEN-LOOP Project, due to the use of non-bio-based materials as raw materials. Between the two-novel bio-based solutions, the one with cork in the composition has a lower sum of impacts than the one with biodegradable bioplastics only.

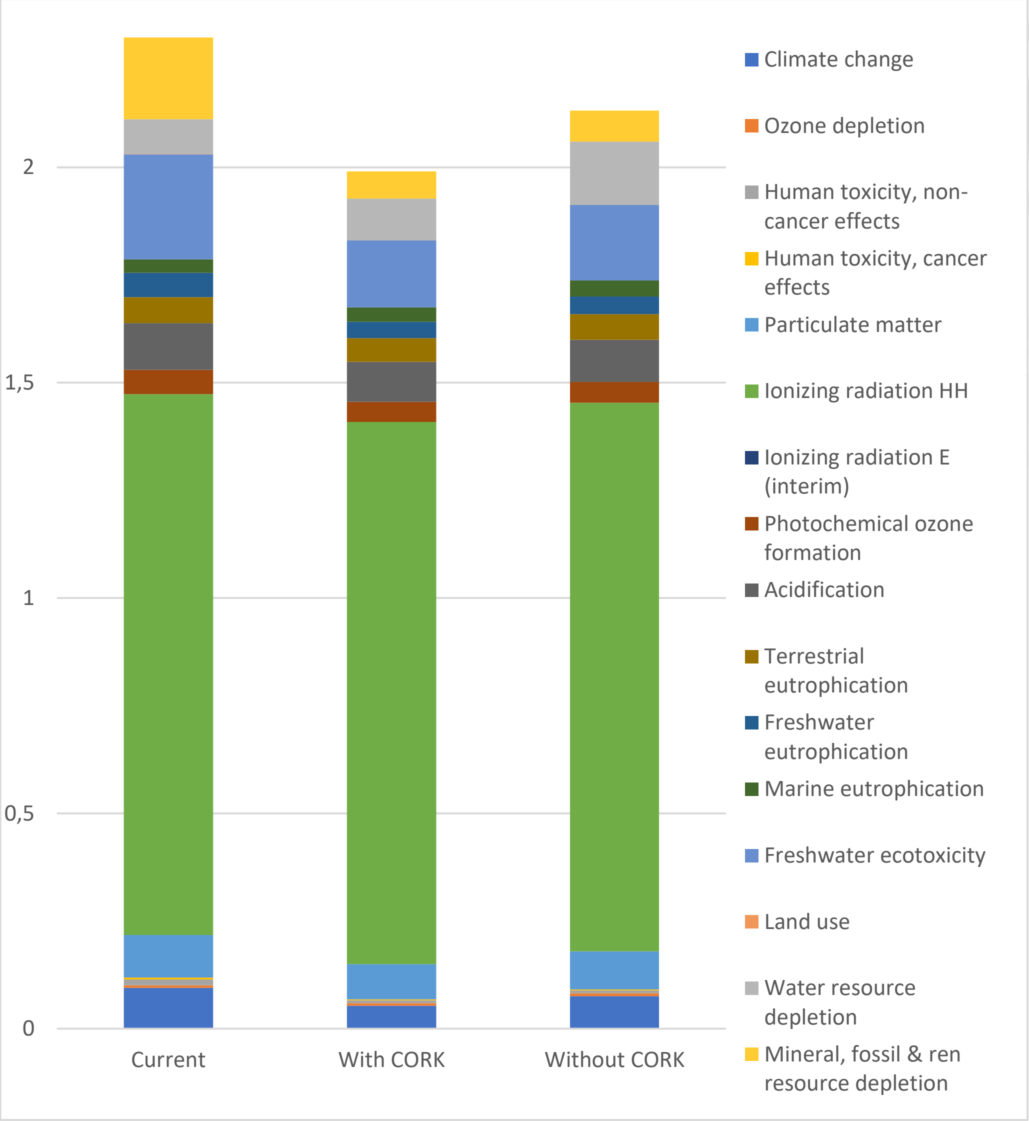

Figure 59. Environmental impacts by Impact categories (mPt) of WP4 scenarios.

To compare the Climate change in kg CO_2 eq category for each scenario, see the Figure 60, which again shows, in line with Figure 59, that the use of current materials produces a carbon footprint almost twice as large as the more environmentally friendly cork-based mix.

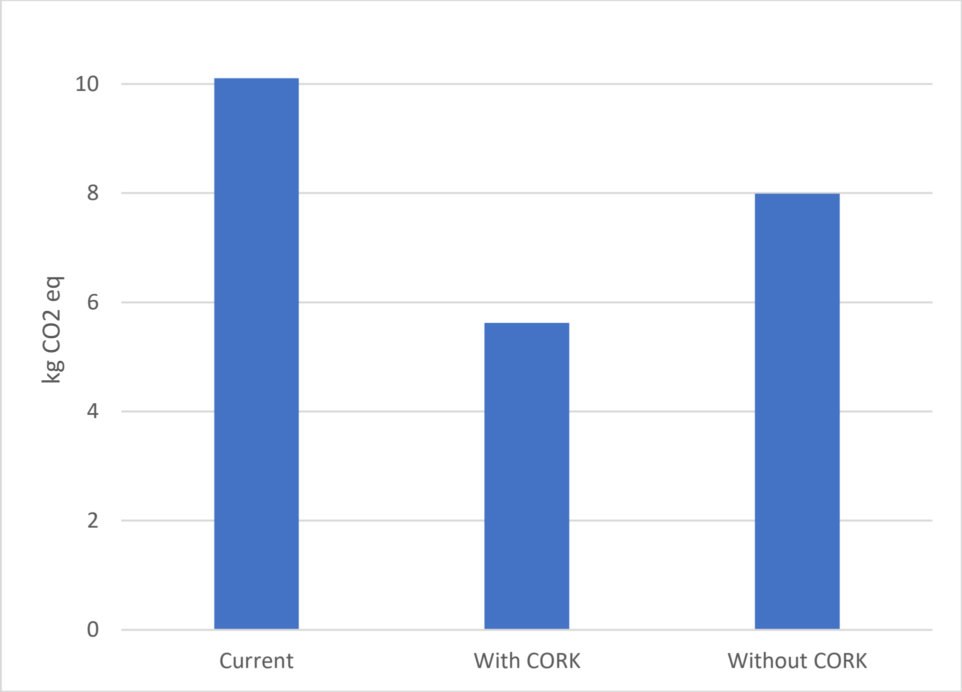

Figure 60. Climate change/Carbon footprint (kg CO2 eq) for WP4 scenarios.

As it is showed in Table 98, the Climate change in the wCORK scenario from WP4 has decreased almost a 43%. In the other GREEN-LOOP Project scenario, the w/oCORK, has decreased a 18%. This huge difference may be for using the biobased material instead of the only use of biodegradable bioplastics.

Table 98. Environmental impact categories for WP4.

Impact categories	Unit	Current	wCORK	w/oCORK
Climate change	mPt	9.79	5.63	7.99
Ozone depletion	mPt	$1.06\cdot10^{-6}$	$1.20\cdot10^{-6}$	$1.25\cdot10^{-6}$
Human toxicity, non-cancer effects	mPt	$1.48\cdot10^{-8}$	$1.42\cdot10^{-6}$	$1.53\cdot10^{-8}$
Human toxicity, cancer effects	mPt	$4.39\cdot10^{-10}$	$4.76\cdot10^{-10}$	$5.27\cdot10^{-10}$
Particulate matter	mPt	0.0065	0.0062	0.0067
Ionizing radiation HH	mPt	4.56	4.55	4.60
Ionizing radiation E (interim)	mPt	$1.27\cdot10^{-5}$	$1.28\cdot10^{-5}$	$1.30\cdot10^{-5}$
Photochemical ozone formation	mPt	0.033	0.031	0.033
Acidification	mPt	0.079	0.079	0.083
Terrestrial eutrophication	mPt	0.13	0.13	0.15
Freshwater eutrophication	mPt	0.0039	0.0037	0.0040

Impact categories	Unit	Current	wCORK	w/oCORK
Marine eutrophication	mPt	0.013	0.015	0.017
Freshwater ecotoxicity	mPt	8.26	8.74	9.84
Land use	mPt	11.99	24.90	21.37
Water resource depletion	mPt	0.062	0.099	0.15
Mineral, fossil & ren resource depletion	mPt	0.00023	0.00018	0.00021

4.3.3. Wood composite manufacture

Figure 61 shows the carbon footprint for all the mixtures inside the WP5, including the current manufacturing. In this figure, it is demonstrated that the MIX1 is the most environmentally friendly mixture, while the MIX3 is the least environmentally friendly, in terms of Carbon footprint (kg CO_2 eq). The different quantities for each mixture are collected in Table 77.

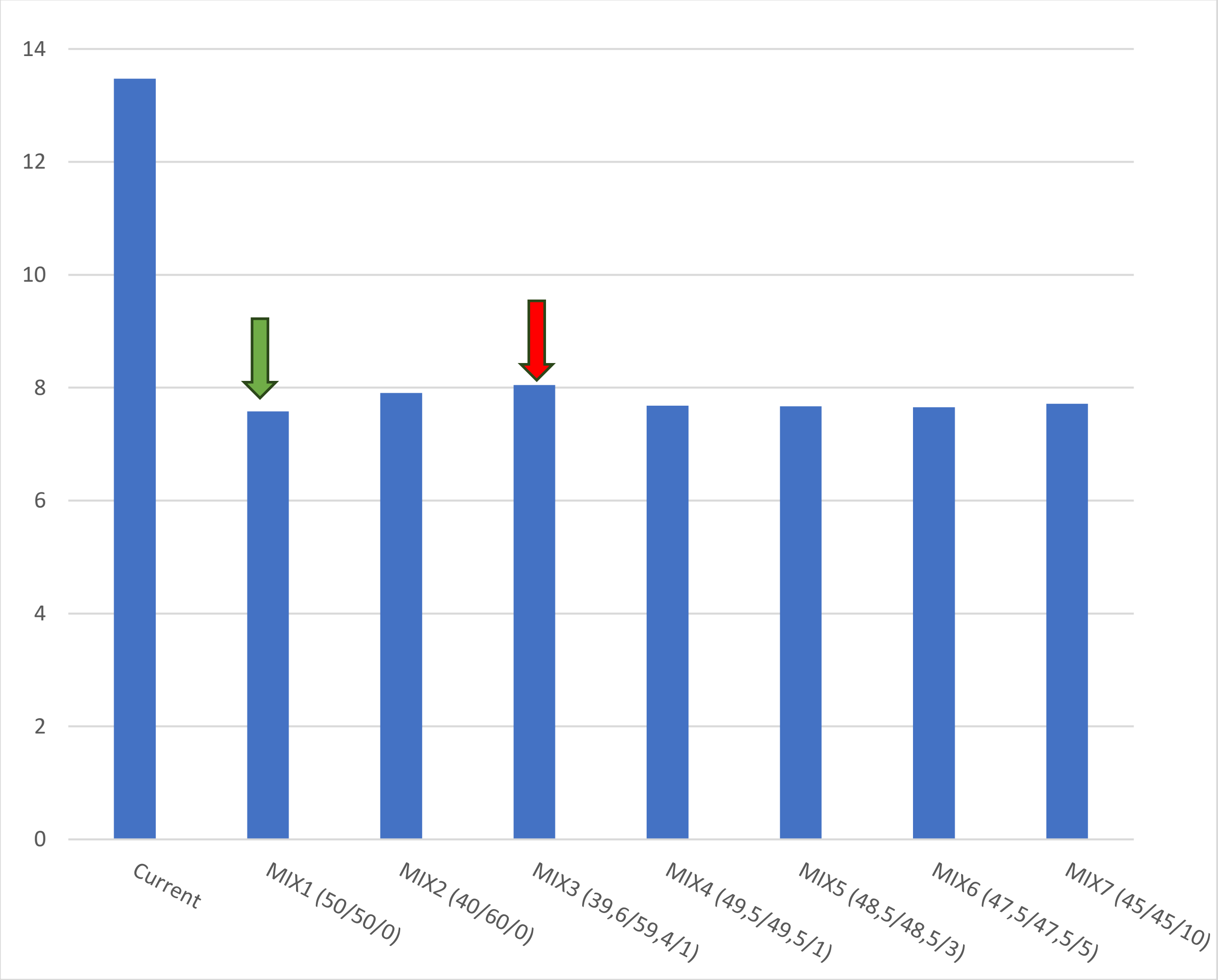

Figure 61. Climate change/Carbon footprint (kg CO2 eq) for WP5 mixtures, in blankets composition of each material.

Finally, Figure 62 shows the process contribution for the three selected scenarios, illustrating how the raw materials impact from the current situation are much higher than the other two GREEN-LOOP scenarios. In MIX1 and MIX3, the energy consumption is the main impact. Between these two options, the MIX1 has a slightly lower impact in raw materials than the other bio-based one, which would be even more beneficial.

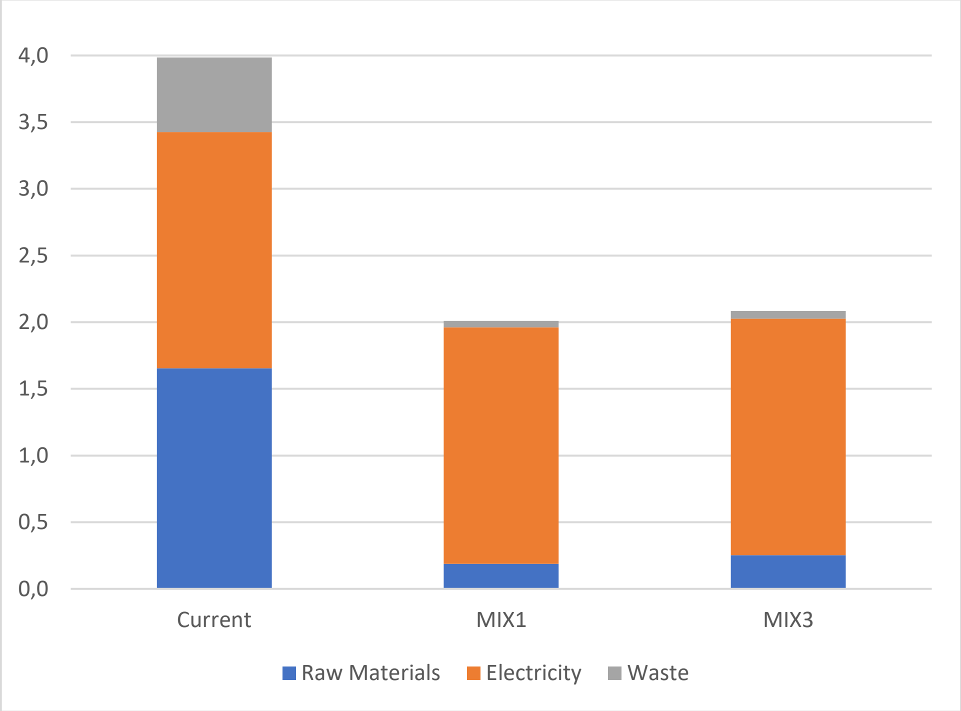

Figure 62. Impacts for process contribution (mPt) for WP5 scenarios.

Table 99 shows that in almost all the impact categories the new mixtures are lower than the current reference scenario. For the *Climate change* impact, the value for MIX1 has decrease a 44%, and for MIX is a 40% lower than the reference value. Regarding the *Mineral, fossil & ren resource depletion* impact, the reduction value is 95% for mixture 1 and 94% for mixture 2.

Table 99. Environmental impact categories for WP5.

Impact categories	Unit	Current	MIX1	MIX3
Climate change	mPt	0.127	0.0715	0.0759
Ozone depletion	mPt	0.00773	0.00693	0.00757
Human toxicity, non-cancer effects	mPt	0.0222	0.00611	0.00647
Human toxicity, cancer effects	mPt	0.00674	0.00589	0.00587
Particulate matter	mPt	0.144	0.0917	0.0993
Ionizing radiation HH	mPt	1.35	1.28	1.30
Ionizing radiation E (interim)	mPt	0	0	0
Photochemical ozone formation	mPt	0.0783	0.0476	0.0502
Acidification	mPt	0.131	0.0956	0.102
Terrestrial eutrophication	mPt	0.0741	0.0559	0.0601

Impact categories	Unit	Current	MIX1	MIX3
Freshwater eutrophication	mPt	0.0948	0.0386	0.0411
Marine eutrophication	mPt	0.0408	0.0340	0.0380
Freshwater ecotoxicity	mPt	0.497	0.151	0.161
Land use	mPt	0.000257	0.000283	0.000324
Water resource depletion	mPt	0.163	0.0585	0.0589
Mineral, fossil & ren resource depletion	mPt	1.25	0.0676	0.0790

4.4. LCC results

4.4.1. Bio-rubber manufacture

In line with LCC analysis, the costing regarding three scenarios in WP3 is shown in Table 100. For the results plotted in Figure 63, the Labour cost has not taken into account, because it is a non-representative due to the low TRL level of the process at this stage (TRL4). At a higher industrial scale, it is anticipated that the labour cost will not be equivalent to the process hour duration due to the high level of process automation.

So, in these conditions, the main economic impact is the purchasing of Raw Materials, with a value of Net Present Value (NPV) around 40-50% in all scenarios, followed by the Indirect manufacture cost (between 22-30% of the NPV for each different scenario); that includes the equipment cost. As it was mentioned above, the consumption would not be comparable for a lab scale process against an industrial one. Hence, the energy consumption for BRP1 and Current manufacturing is assumed to be equivalent for the same scale. One part of the Indirect cost is calculated as 5% of direct cost, and the Manufacture profits as the 7% of direct cost, according to the assumptions explained in section 2.2.1. Finally, the Environmental externalities are calculated with SIMAPRO software and the Environmental Prices database.

Table 100. Cost table for WP3.

Data for 1kg of:		BRP1	BRP2	Current RP
Raw materials	RM purchase	42.22 €	42.22 €	42.23 €
Direct manufacture cost	Energy	21.09 €	15.73 €	21.09 €
	Labour cost	4.235.10 €	3.041.15 €	4.235.10 €
Indirect manufacture cost	Waste management	2.79 €	2.79 €	2.79 €
	5% direct	1.05 €	0.79 €	1.05 €
	Equipment cost	28.37 €	15.01 €	28.37 €
Manufacture profits	7% direct	297.93 €	213.98 €	297.93 €
Environmental cost	Environmental Prices V1.00 - SIMAPRO	7.75 €	6.84 €	8.15 €
Component cost	TOTAL	**4.636.31 €**	**3.338.51 €**	**4.636.72 €**

The use of these natural resources has a slightly lower NPV impact in comparison with the synthetic rubber during the last step of the process. The use of sonicator with the second reactor of 0.8L in BRP2 is beneficial (environmentally and economically) for this GREEN-LOOP manufacturing. Also, it is important to mention that a reduction in the environmental impacts produce a reduction of the Environmental Externalities costs, this second scenario has the lowest economic impact.

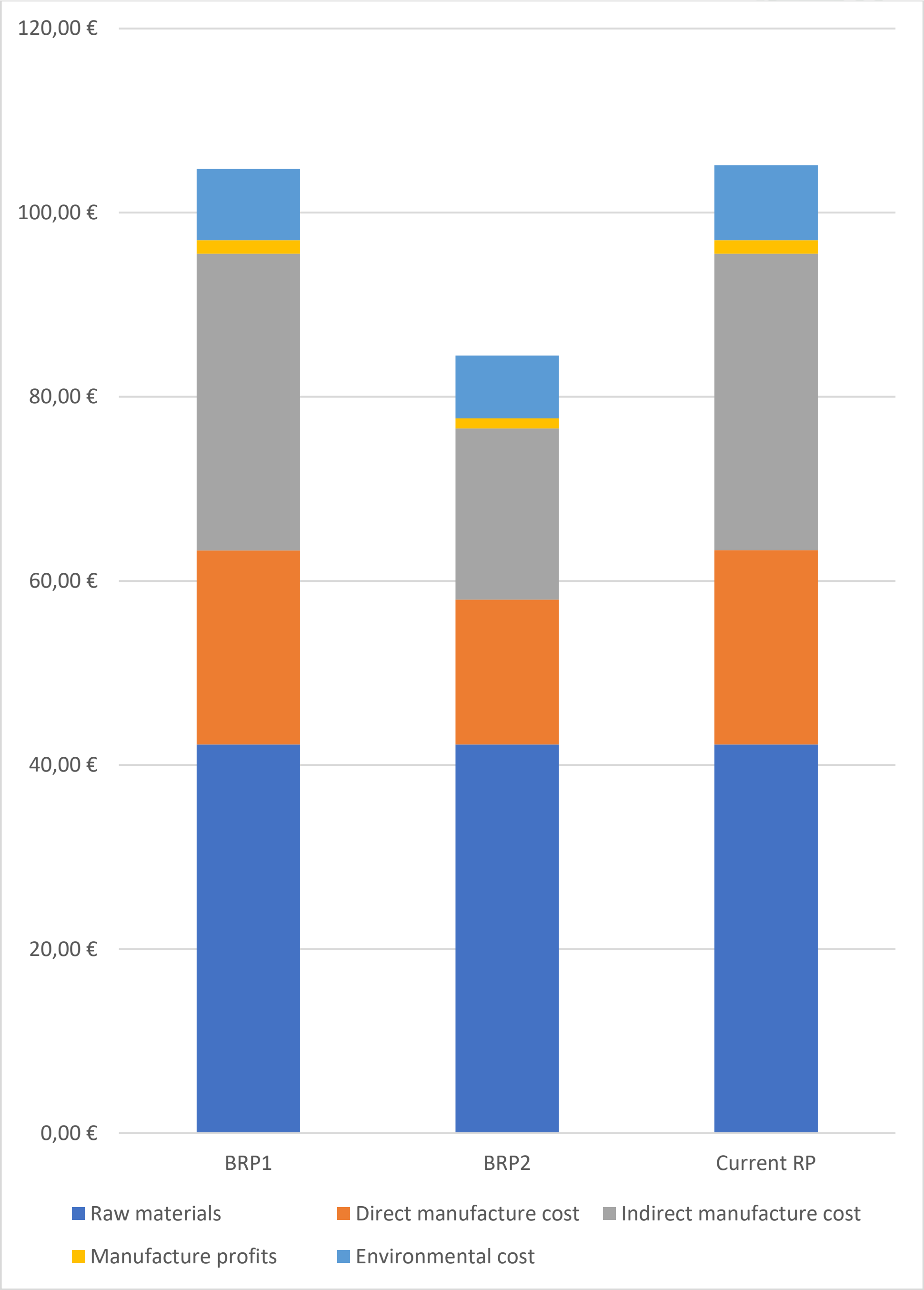

Figure 63. Life Cycle Costing (LCC) of WP3 scenarios.

4.4.2. Bioplastic manufacture

In the LCC analysis, all the economic data obtained for the three scenarios in WP4 is summarised in Table 101. In this case the Labour cost is included in Direct cost because it is not high as in the previous case. Still, these costs are the main impact detected, but it is considered a more realistic situation due to it is not a very high value in comparison with the rest of the values; it is more balanced across the whole LCC. In the case Labour cost was not taken into account, the raw materials purchasing would be the main impact in the two GREEN-LOOP scenarios, while in the current situation would be the environmental costs due to the no-renewable materials used in this scenario. The info from this Table is reflected in Figure 64. The highest NPV is from the scenario without cork because the raw materials and the environmental externalities have more economic impact in this scenario than the other one with the bio-based material. The price of this biodegradable material is more expensive than the current ones used, namely, aluminium and Low-Density Polyethylene (LDPE). The sum of economic impacts is lower in the current scenario because nowadays the plastic market is well established around the world, with lower prices than the biodegradable options. Even if Environmental externalities are very high for current materials, it does not compensate for the price difference in raw materials.

Table 101. Cost table for WP4.

Data for 1kg of:		wCORK	w/oCORK	Current
Raw materials	RM purchase	12.10 €	12.52 €	1.97 €
Direct manufacture cost	Energy	4.28 €	4.28 €	4.28 €
	Labour cost	56.39 €	56.39 €	56.39 €
Indirect manufacture cost	Waste management	0.00 €	0.00 €	0.00 €
	5% direct	3.03 €	3.03 €	3.03 €
	Equipment cost	0.97 €	0.97 €	0.97 €
Manufacture profits	7% direct	4.25 €	4.25 €	4.25 €
Environmental cost	Environmental Prices V1.00 - SIMAPRO	2.67 €	3.10 €	6.38 €
Component cost	**TOTAL**	**83.69 €**	**84.54 €**	**77.27 €**

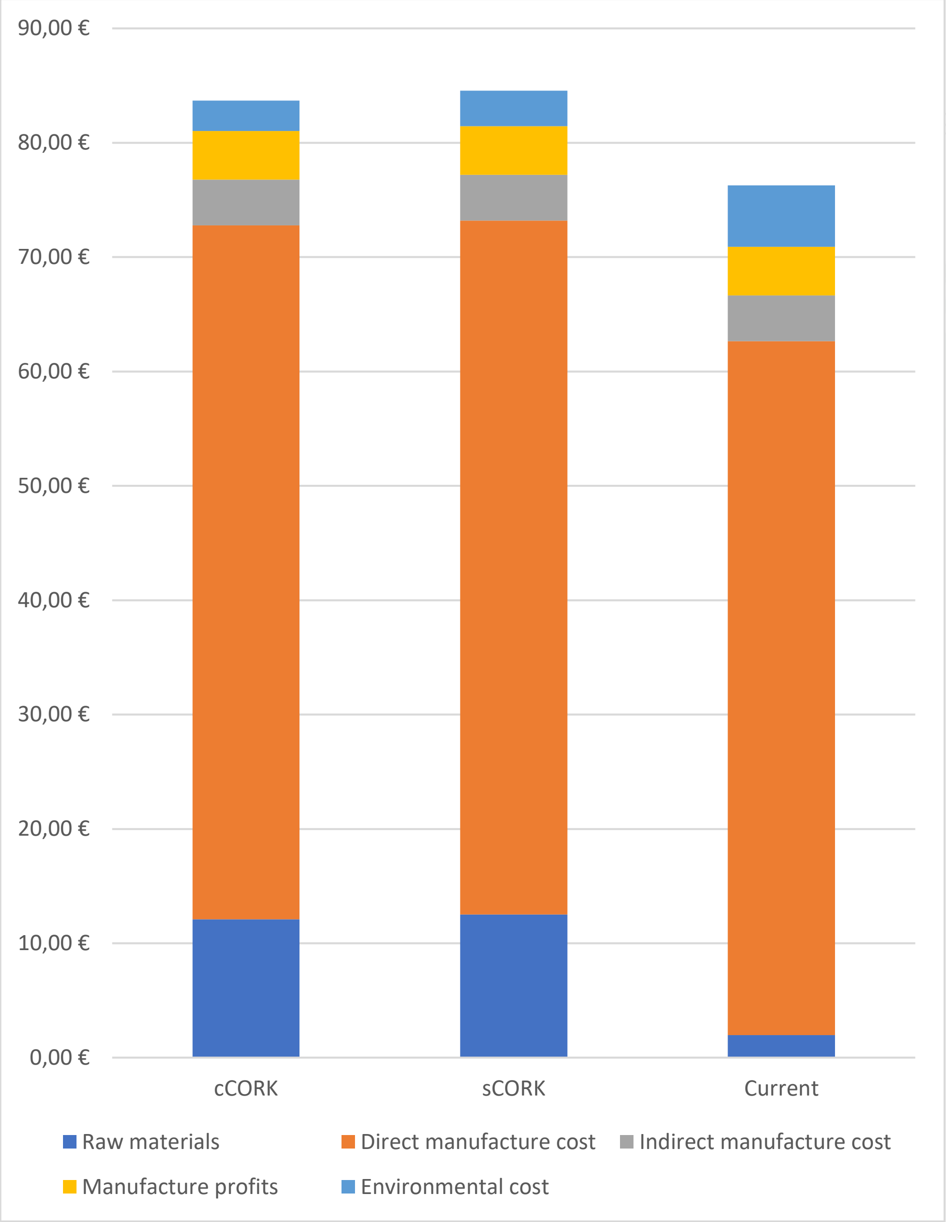

Figure 64. Life Cycle Costing (LCC) for WP4 scenarios.

4.4.3. Wood composites manufacture

For the LCC analysis in this WP, all the costs associated with these scenarios are collected on Table 102. Making the same considerations as in the previous WPs, the NPV for Raw materials with the current scenario (41.91%) is almost the double of the presented with MIX1 materials (21.64%), and a 10% higher than MIX3 (31.34%). For all scenarios, the main impact will be the direct manufacture cost, representing a 67.80% for the MIX1, a 59% with MIX3 and finally, 46.59% in the current manufacturing. All this info is represented in Figure 65.

Table 102. Cost table for WP5.

Data for 1kg of:		MIX1	MIX3	Current
Raw materials	RM purchase	28.63 €	47.66 €	80.70 €
Direct manufacture cost	Energy	13.88 €	13.88 €	13.88 €
	Labour cost	75.83 €	75.83 €	75.83 €
Indirect manufacture cost	Waste management	-0.07 €	-0.13 €	0.16 €
	5% direct	4.49 €	4.49 €	4.49 €
	Equipment cost	0.84 €	0.84 €	0.84 €
Manufacture profits	7% direct	6.28 €	6.28 €	6.28 €
Environmental cost	Environmental Prices V1.00 - SIMAPRO	2.45 €	3.20 €	10.38 €
Component cost	**TOTAL**	**132.33 €**	**152.05 €**	**192.55 €**

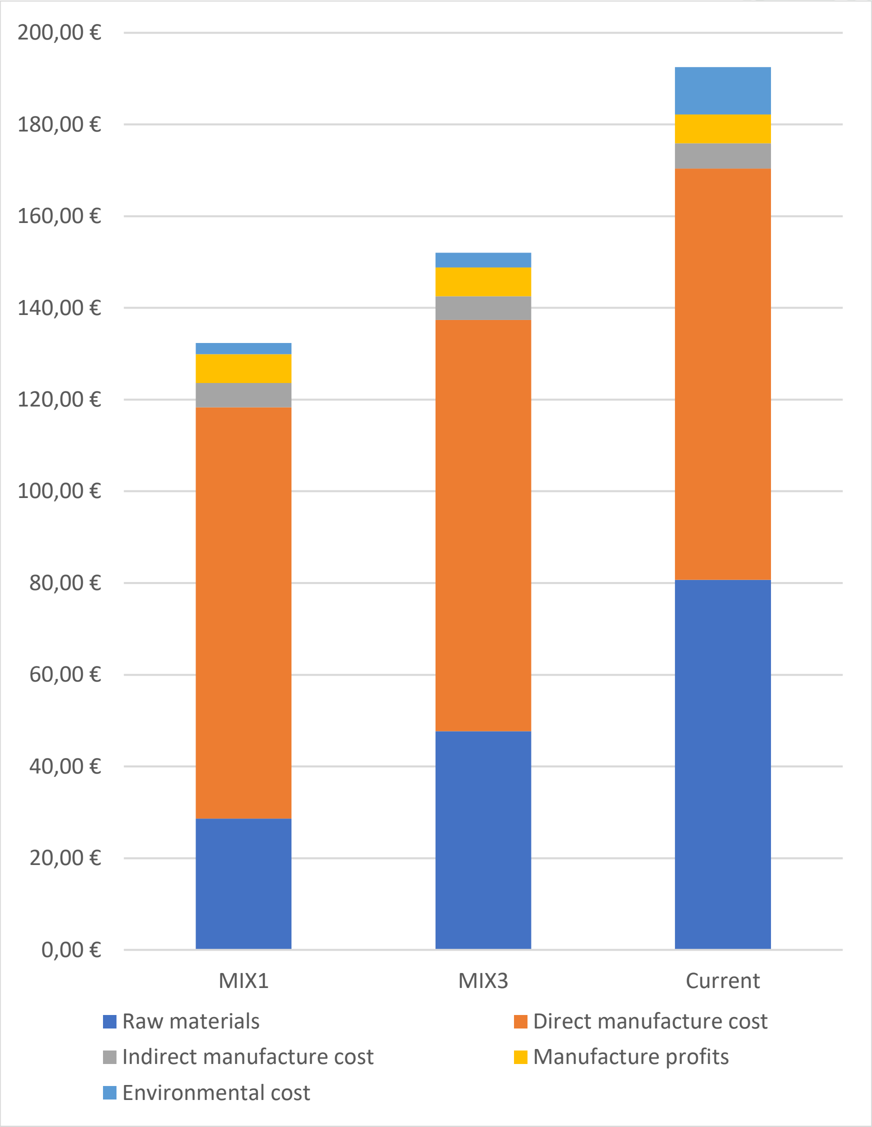

Figure 65. Life Cycle Costing (LCC) for WP5 scenarios.

5. Conclusions

In the present Deliverable 2.2, the energy and exergy analyses, as well as the life cycle analysis were carried out. They were developed for the three different value chains developed in GREEN-LOOP project during the las two years (M1-M24), namely bio rubber manufacturing (developed by NCC in WP3), bioplastic manufacturing (developed by LBRT in WP4) and wood composite manufacturing (developed by FHF in WP5). The equipment with the highest consumption, as well as the irreversibilities and energy resources, have been identified for each process.

At first, a data collection procedure was implemented to gather the contributions of each partner. These contributions are then used to create process flow diagrams (PFDs) for different manufacturing processes. After the questionnaires are validated, they are circulated to seek the necessary information for the establishment of mass and energy balances. The processes are broken down into separate parts, and mass, energy, and exergy balances are calculated for each phase and the complete operations.

The raw materials and conditions of the operations are determined in order to carry out mass balances that are needed to conduct energy and exergy balances. The different equipment used in the processes are identified for the energy balances. The partners are required to provide details pertaining to the power consumption and duration of operation for each equipment utilised in the manufacturing process. An analysis is conducted on the power consumption of devices that perform work or provide and remove energy inside a system. This analysis involves identifying and calculating the different energy contributions that occur at various stages of the processes. With the results obtained in the energy balance, it is possible to conduct an exergy analysis.

The following conclusions can be obtained from the energy and exergy analyses developed in this deliverable:

- **There are three processes in WP3.** In lignin extraction, even though the calculation is not fully accurate due to the lack of the data, it is clear that pulping step is the process that requires the larger amount of energy, as reactors are equipment with huger energy demands. However, the energy lost in pulping step is remarkable. In the rest of the steps of lignin extraction, energy demands are not as large, in some cases even zero. The energy destroyed in the rest of the steps can be considered negligible in comparison with the energy losses in pulping step.
  During rubber functionalisation process, sonication is the step that requires more energy, but compared to the energy required during lignin extraction is practically insignificant. Although the energy requirements are very low, almost all of the energy produced is lost during the process. Only a portion of the energy produced in the heating process is utilised by the system.
  In rubber panel production occur something similar that in rubber functionalisation. Compression moulding and compounding steps requires amounts of energy to be considered, but compared to pulping are insignificant. Energy destroyed comprise almost most of the energy generated during the entire process.
- **In bioplastic manufacturing process developed in WP4,** energy contributions are not well quantified due to the lack of data. However, it is expected that extrusion and injection moulding have larger amounts of energy demands. Also, the energy decoyed during the process would probably be considerably big.

- **Regarding WP5’s wood composites value chain,** the step that involves a greater requirement of energy is compression moulding. Also, as in the rest of the process studied in the Deliverable, most of the energy generated during the process is lost. A portion of the energy is dissipated as heat in mixing, extrusion and compression moulding steps.

Regarding life cycle analysis, the work presented in this Deliverable is a combination of the LCA and LCC analysis, taking into account a current equivalent product in the market and two new bio-based scenarios developed during the GREEN-LOOP Project. This preliminary assessment helps to identify different hotspots in the GREEN-LOOP materials and to propose different actions for improvement, to following the sustainability path in the use of bio-based materials and avoiding the petroleum-based ones.

In reviewing of the results, one of the main important hotspots identified is related to one SSbD criterion: energy efficiency consumption during the production process, due to the long reaction times required at laboratory scale. Therefore, particular attention must be paid to optimizing energy consumption in subsequent development steps:

- **In WP3,** the environmental process impact related to Raw Material for GREENLOOP scenarios (BRP1 And BRP2) is lower than in the current market material due to the use of synthetic rubber instead of natural rubber. Therefore, the use of bio-based materials has a positive environmental impact in the process. In terms of the economic point of view, the main result from the LCC (excluding labour costs) is the conclusion that the BRP2 scenario is the most favourable due to its lower energy consumption.

- **In WP4,** where two-novel bio-based solutions are compared, the one with cork in the composition has a lower sum of impacts than the other with biodegradable bioplastics only. This result remarks the importance of the use of bio-based materials over other alternatives. On the other hand, the current reference situation has a slightly lower NPV in comparison with the two mixtures developed in GREEN-LOOP Project. This is mainly due to the fact that nowadays plastics market price is lower than the alternative biodegradable options, but minor improvements in this trend would make these options to be competitive with the plastic-based option. Nevertheless, the environmental externalities are higher for current market options, due to the impacts that these materials (aluminium and LDPE) generate to the environment.

- **In WP5,** the bio-based solution with a higher quantity of wood (50% MIX1 vs. 39.6% MIX3) has the lowest environmental and cost impact due to a bigger used of bio-based materials. The analysis against the metallic material has almost twice of the environmental impact versus the bio-based mixtures developed in GREEN-LOOP Project, providing the benefits that this innovation could have for the wood composites.

6. Action plan for further analysis

The results obtained from these analyses are the pillars to continue with the different assessments, due to this screening results will be able to detect different hotspots in every value chain, as the use of determined raw materials, the electricity consumption, or some wastes or emissions that affect the environment or the human health.

The strategy to continue in line in these analyses (including sLCA) is to align T2.2 and T2.3 in the upscaling process and validation phase, including industrial relevant data from the WP6. The next deliverable will contain final results for LCA, LCC, sLCA and energy and exergy analyses taking into account the whole value chain of each technical WP manufacturing (bio-rubber panels, bioplastic closures and wood composites). Recyclability, reuse, refurbish, or waste reduction are some KPIs set up in Task T1.3: “Validation KPI’s definition”, which will be studied in this final report. As a living document, the LCI will be continually updated. Energy and exergy analyses will be evaluated in the upscaled manufacturing process. Considering the changes in parameters and configurations in the upscaled process, suggestions of improvements will be made. Irreversibilities, losses and final costs of the products will also be assessed.

These updates will be taken into account and reflected in D2.3 at the end of the project, in M36. WP3, WP4 and WP5 will use this deliverable as an output for decision making in the remainder of the project, during the escalation of the various processes in WP6.

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Annex 1: Datasets for energy and exergy balance

Table 103. Energy and exergy balance WP3 Dataset.

Process	Step	Parameter	Value	Unit
Lignin extraction	Pulping	$m_{biomass}$ (Lignocellulosic biomass mass)	138.95	g
		V_{water} (Water volume)	0.69	L
		m_{Na_2S} (Sodium sulfide mass)	6.94	g
		m_{NaOH} (Sodium hydroxide mass)	23.61	g
		$\%_{cellulose}$ (Cellulose percentage in biomass)	42	%
		$\%_{hemicellulose}$ (Hemicellulose percentage in biomass)	22	%
		$\%_{lignin}$ (Lignin percentage in biomass)	24	%
		$T_{pulping}$ (Temperature of pulping process)	448	K
		$E_{pulping}$ (Power reactor)	3.68	kW
		$t_{pulping}$ (Time of pulping process)	180	min
	Filtration 1	$m_{cellulose}$ (Filtrated cellulose mass)	58.36	g
		$T_{filtration\ 1}$ (Temperature of filtration 1 process)	298	K
	Acidification	$V_{H_2SO_4,15\%}$ (Sulfuric acid 15% volume)	0.1	L
		$T_{acidification}$ (Temperature of acidification process)	298	K
	Filtration 2	$V_{acid\ liquor}$ (Acid liquor volume)	0.48	L
		$\rho_{acid\ liquor}$ (Acid liquor density)	1.1	g/cm^3
		$T_{filtration\ 2}$ (Temperature of filtration 2 process)	298	K
	Washing	$V_{H_2SO_4,5\%,clean}$ (Sulfuric acid 5% clean volume)	0.21	L
		$V_{H_2SO_4,5\%,dirty}$ (Sulfuric acid 5% dirty volume)	0.17	L
		$\rho_{H_2SO_4,5\%,dirty}$ (Sulfuric acid 5% dirty density)	1.1	g/cm^3
		$T_{washing}$ (Temperature of washing process)	298	K
	Drying	$V_{moisture}$ (Moisture volume)	0.03	L
		m_{lignin} (Lignin powder mass)	25	g
		T_{drying} (Temperature of drying process)	298	K
Rubber functionalisation	Sonication	$m_{rubber\ crumb}$ (Rubber crumb mass)	100	g
		$E_{sonicator}$ (Power sonicator)	0.1	kW
		$t_{pulping}$ (Time of pulping process)	20	min
		$T_{sonication}$ (Temperature of sonication process)	298	K
	Heating	T_{drying} (Temperature of heating process)	453	K
	Filtration	m_{DES} (Filtrated and recovered DES mass)	2000	g

Process	Step	Parameter	Value	Unit
		m_{wastes} (Wastes mass)	20	g
		$m_{functionalised\ rubber}$ (Functionalised rubber mass)	80	g
		$T_{filtration}$ (Temperature of filtration process)	298	K
Rubber and panel production	Compounding	$m_{lignin\ powder}$ (Lignin powder mass)	25	g
		$m_{devulcanised\ rubber}$ (Devulcanized rubber mass)	80	g
		$m_{natural\ rubber}$ (Natural rubber mass)	20	g
		m_{ZnO} (Zinc oxide mass)	5	g
		$m_{stearic\ acid}$ (Stearic acid mass)	1	g
		$m_{MBTS-75}$ (MBTS-75 mass)	0.5	g
		$m_{sulphur}$ (Sulphur mass)	2.5	g
		$T_{compounding}$ (Temperature of compounding process)	313	K
		$E_{compounding}$ (Power mixer)	0.313	kW
		$t_{compounding}$ (Time of compounding process)	7	min
		$m_{compounding\ losses}$ (Compounding losses mass)	6.7	g
	Cooling	$T_{cooling}$ (Temperature of cooling process)	298	K
	Cutting	$T_{cutting}$ (Temperature of cutting process)	298	K
	Compression moulding	$m_{compression\ moulding\ losses}$ (Compression moulding losses mass)	6.4	g
		$T_{compression\ moulding}$ (Temperature of compression moulding process)	433	K
		$E_{compression\ moulding}$ (Power press)	0.283	kW
		$t_{compression\ moulding}$ (Time of compression moulding process)	30	min
	Machining	$m_{machining\ losses}$ (Machining losses mass)	6	g
		$T_{machining}$ (Temperature of machining process)	298	K

Table 104. Energy and exergy balance WP4 Dataset.

Step	Parameter	Value	Unit
Dispenser	$m_{dispenser}$ (Dispensed mass)	10	kg
	$\%_{PHBH}$ (PHBH percentage in dispensed mass)	66.7	%
	$\%_{PLA}$ (PLA percentage in dispensed mass)	13.3	%
	$\%_{cork}$ (Cork percentage in dispensed mass)	20	%
	$T_{preheating}$ (Temperature of preheated samples)	328	K
Extrusion	$E_{extruder}$ (Power extruder)	10.95	kW/kg
	$T_{extruder}$ (Temperature of extrusion process)	443	K

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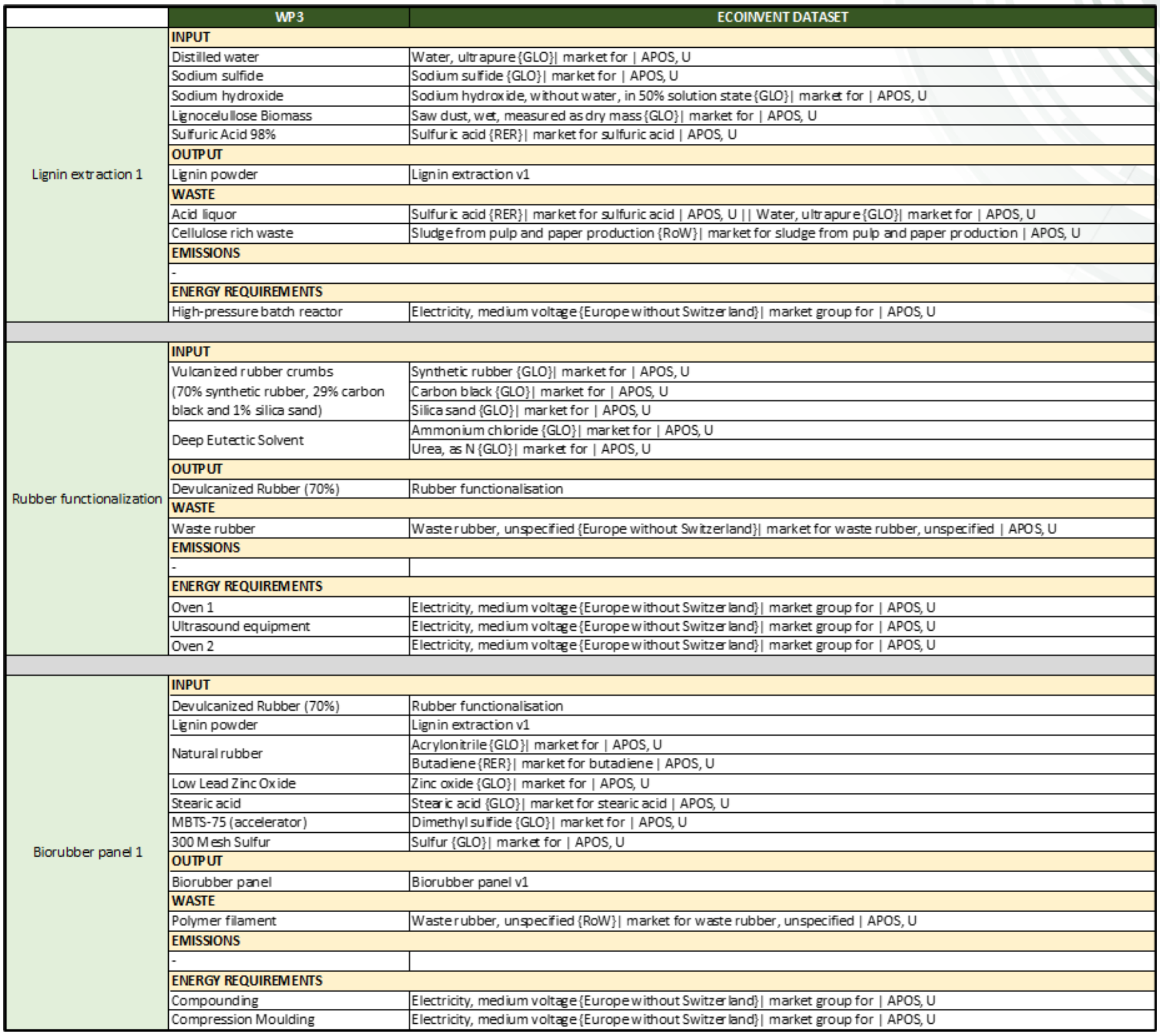
Step	Parameter	Value	Unit
Injection moulding	$E_{injection\ moulding}$ (Power injection moulding machine)	4	kW/kg
	$T_{injection\ moulding}$ (Temperature of injection moulding process)	298	K

Table 105. Energy and exergy balance WP5 Dataset.

Step	Parameter	Value	Unit
Mixing	$m_{bio-polymer}$ (Bio-polymer mass)	1000	g
	m_{fibers} (Fibers mass)	430	g
	T_{mixing} (Temperature of mixing process)	473	K
	E_{mixing} (Power mixer)	5	kW
	t_{mixing} (Time of mixing process)	30	min
Extrusion	$T_{estrusion}$ (Temperature of extrusion process)	473	K
	$E_{extrusion}$ (Power extruder)	1.5	kW
	$t_{extrusion}$ (Time of extrusion process)	90	min
Kneading	$T_{kneading}$ (Temperature of kneading process)	298	K
	$E_{kneading}$ (Power kneader)	1.1	kW
	$t_{kneading}$ (Time of kneading process)	60	min
Compression moulding	$\%_{bio-polymer\ recovered}$ (Bio-polymer recovered percentage)	8.33	%
	$\%_{fibers\ recovered}$ (Fibers recovered percentage)	8.33	%
	$T_{kneading}$ (Temperature of kneading process)	473	K
	$E_{kneading}$ (Power kneader)	10	kW
	$t_{kneading}$ (Time of kneading process)	40	min

Annex 2: Datasets for LCA and LCC in WP3

Table 106. Dataset used for WP3 – BRP1



	WP3	ECOINVENT DATASET
Lignin extraction 1	**INPUT**	
	Distilled water	Water, ultrapure {GLO}| market for | APOS, U
	Sodium sulfide	Sodium sulfide {GLO}| market for | APOS, U
	Sodium hydroxide	Sodium hydroxide, without water, in 50% solution state {GLO}| market for | APOS, U
	Lignocelullose Biomass	Saw dust, wet, measured as dry mass {GLO}| market for | APOS, U
	Sulfuric Acid 98%	Sulfuric acid {RER}| market for sulfuric acid | APOS, U
	OUTPUT	
	Lignin powder	Lignin extraction v1
	WASTE	
	Acid liquor	Sulfuric acid {RER}| market for sulfuric acid | APOS, U || Water, ultrapure {GLO}| market for | APOS, U
	Cellulose rich waste	Sludge from pulp and paper production {RoW}| market for sludge from pulp and paper production | APOS, U
	EMISSIONS	
	-	
	ENERGY REQUIREMENTS	
	High-pressure batch reactor	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
Rubber functionalization	**INPUT**	
	Vulcanized rubber crumbs (70% synthetic rubber, 29% carbon black and 1% silica sand)	Synthetic rubber {GLO}| market for | APOS, U
		Carbon black {GLO}| market for | APOS, U
		Silica sand {GLO}| market for | APOS, U
	Deep Eutectic Solvent	Ammonium chloride {GLO}| market for | APOS, U
		Urea, as N {GLO}| market for | APOS, U
	OUTPUT	
	Devulcanized Rubber (70%)	Rubber functionalisation
	WASTE	
	Waste rubber	Waste rubber, unspecified {Europe without Switzerland}| market for waste rubber, unspecified | APOS, U
	EMISSIONS	
	-	
	ENERGY REQUIREMENTS	
	Oven 1	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Ultrasound equipment	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Oven 2	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
Biorubber panel 1	**INPUT**	
	Devulcanized Rubber (70%)	Rubber functionalisation
	Lignin powder	Lignin extraction v1
	Natural rubber	Acrylonitrile {GLO}| market for | APOS, U
		Butadiene {RER}| market for butadiene | APOS, U
	Low Lead Zinc Oxide	Zinc oxide {GLO}| market for | APOS, U
	Stearic acid	Stearic acid {GLO}| market for stearic acid | APOS, U
	MBTS-75 (accelerator)	Dimethyl sulfide {GLO}| market for | APOS, U
	300 Mesh Sulfur	Sulfur {GLO}| market for | APOS, U
	OUTPUT	
	Biorubber panel	Biorubber panel v1
	WASTE	
	Polymer filament	Waste rubber, unspecified {RoW}| market for waste rubber, unspecified | APOS, U
	EMISSIONS	
	-	
	ENERGY REQUIREMENTS	
	Compounding	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Compression Moulding	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U

Table 107. Dataset used for WP3 – BRP2.

	WP3	ECOINVENT DATASET
Lignin extraction 2	**INPUT**	
	Distilled water	Water, ultrapure {GLO}| market for | APOS, U
	Sodium sulfide	Sodium sulfide {GLO}| market for | APOS, U
	Sodium hydroxide	Sodium hydroxide, without water, in 50% solution state {GLO}| market for | APOS, U
	Lignocelullose Biomass	Saw dust, wet, measured as dry mass {GLO}| market for | APOS, U
	Sulfuric Acid 98%	Sulfuric acid {RER}| market for sulfuric acid | APOS, U
	OUTPUT	
	Lignin powder	Lignin extraction v2
	WASTE	
	Acid liquor	Sulfuric acid {RER}| market for sulfuric acid | APOS, U || Water, ultrapure {GLO}| market for | APOS, U
	Cellulose rich waste	Sludge from pulp and paper production {RoW}| market for sludge from pulp and paper production | APOS, U
	EMISSIONS	
	-	
	ENERGY REQUIREMENTS	
	Ultrasound sonicator	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	High-pressure batch reactor	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
Rubber functionalization	**INPUT**	
	Vulcanized rubber crumbs (70% synthetic rubber, 29% carbon black and 1% silica sand)	Synthetic rubber {GLO}| market for | APOS, U
		Carbon black {GLO}| market for | APOS, U
		Silica sand {GLO}| market for | APOS, U
	Deep Eutectic Solvent	Ammonium chloride {GLO}| market for | APOS, U
		Urea, as N {GLO}| market for | APOS, U
	OUTPUT	
	Devulcanized Rubber (70%)	Rubber functionalisation
	WASTE	
	Waste rubber	Waste rubber, unspecified {Europe without Switzerland}| market for waste rubber, unspecified | APOS, U
	EMISSIONS	
	-	
	ENERGY REQUIREMENTS	
	Oven 1	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Ultrasound equipment	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Oven 2	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
Biorubber panel 2	**INPUT**	
	Devulcanized Rubber (70%)	Rubber functionalisation
	Lignin powder	Lignin extraction v2
	Natural rubber	Acrylonitrile {GLO}| market for | APOS, U
		Butadiene {RER}| market for butadiene | APOS, U
	Low Lead Zinc Oxide	Zinc oxide {GLO}| market for | APOS, U
	Stearic acid	Stearic acid {GLO}| market for stearic acid | APOS, U
	MBTS-75 (accelerator)	Dimethyl sulfide {GLO}| market for | APOS, U
	300 Mesh Sulfur	Sulfur {GLO}| market for | APOS, U
	OUTPUT	
	Biorubber panel	Biorubber panel v2
	WASTE	
	Polymer filament	Waste rubber, unspecified {RoW}| market for waste rubber, unspecified | APOS, U
	EMISSIONS	
	-	
	ENERGY REQUIREMENTS	
	Compounding	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Compression Moulding	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U

Table 108. Dataset used for WP3 – Current panel.

	WP3	ECOINVENT DATASET
Lignin extraction 1	**INPUT**	
	Distilled water	Water, ultrapure {GLO}| market for | APOS, U
	Sodium sulfide	Sodium sulfide {GLO}| market for | APOS, U
	Sodium hydroxide	Sodium hydroxide, without water, in 50% solution state {GLO}| market for | APOS, U
	Lignocelullose Biomass	Saw dust, wet, measured as dry mass {GLO}| market for | APOS, U
	Sulfuric Acid 98%	Sulfuric acid {RER}| market for sulfuric acid | APOS, U
	OUTPUT	
	Lignin powder	Lignin extraction v1
	WASTE	
	Acid liquor****	Sulfuric acid {RER}| market for sulfuric acid | APOS, U || Water, ultrapure {GLO}| market for | APOS, U
	Cellulose rich waste	Sludge from pulp and paper production {RoW}| market for sludge from pulp and paper production | APOS, U
	EMISSIONS	
	-	
	ENERGY REQUIREMENTS	
	High-pressure batch reactor	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
Rubber functionalization	**INPUT**	
	Vulcanized rubber crumbs (70% synthetic rubber, 29% carbon black and 1% silica sand)	Synthetic rubber {GLO}| market for | APOS, U
		Carbon black {GLO}| market for | APOS, U
		Silica sand {GLO}| market for | APOS, U
	Deep Eutectic Solvent (stay in system)	Ammonium chloride {GLO}| market for | APOS, U
		Urea, as N {GLO}| market for | APOS, U
	OUTPUT	
	Devulcanized Rubber (70%)	Rubber functionalisation
	WASTE	
	Waste rubber	Waste rubber, unspecified {Europe without Switzerland}| market for waste rubber, unspecified | APOS, U
	EMISSIONS	
	-	
	ENERGY REQUIREMENTS	
	Oven 1	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Ultrasound equipment	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Oven 2	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
Current rubber panel	**INPUT**	
	Devulcanized Rubber (70%)	Rubber functionalisation
	Lignin powder	Lignin extraction v1
	Virgin rubber	Synthetic rubber {GLO}| market for | APOS, U
	Low Lead Zinc Oxide	Zinc oxide {GLO}| market for | APOS, U
	Stearic acid	Stearic acid {GLO}| market for stearic acid | APOS, U
	MBTS-75 (accelerator)****	Dimethyl sulfide {GLO}| market for | APOS, U
	300 Mesh Sulfur	Sulfur {GLO}| market for | APOS, U
	OUTPUT	
	Current Panel	Rubber panel current
	WASTE	
	Polymer filament	Waste rubber, unspecified {RoW}| market for waste rubber, unspecified | APOS, U
	EMISSIONS	
	-	
	ENERGY REQUIREMENTS	
	Compounding	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Compression Moulding	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U

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Table 109. Dataset used for WP4 – Bioplastic olive oil closure (with cork).

	WP4	ECOINVENT
Olive oil closures (with CORK)	**INPUT**	
	PHBH	Polyester-complexed starch biopolymer {GLO}| market for | APOS, U
	PLA	Polylactide, granulate {GLO}| market for | APOS, U
	Cork	Cork, raw {GLO}| market for | APOS, U
	OUTPUT	
	Bottle closures	Bioplastic closure + cork
	WASTE	
	-	
	EMISSIONS	
	-	
	ENERGY REQUIREMENTS	
	Hopper loader	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Extruder	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Microwave preheating system	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Deshumidifier	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Injectiong moulding machine	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U

Table 110. Dataset used for WP4 – Bioplastic olive oil closure (without cork).

	WP4	ECOINVENT
Olive oil closures (without CORK)	**INPUT**	
	PHBH	Polyester-complexed starch biopolymer {GLO}| market for | APOS, U
	PLA	Polylactide, granulate {GLO}| market for | APOS, U
	OUTPUT	
	Bottle closures	Bioplastic closure
	WASTE	
	-	
	EMISSIONS	
	-	
	ENERGY REQUIREMENTS	
	Hopper loader	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Extruder	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Microwave preheating system	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Deshumidifier	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Injectiong moulding machine	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U

Table 111. Dataset used for WP4 – Current plastic olive oil closure.

	WP4	ECOINVENT
Current closures	**INPUT**	
	Aluminium	Aluminium alloy, metal matrix composite {GLO}| market for | APOS, U
	LDPE	Polyethylene, low density, granulate {GLO}| market for | APOS, U
	OUTPUT	
	Bottle closures	Plastic olive oil closure
	WASTE	
	-	
	EMISSIONS	
	-	
	ENERGY REQUIREMENTS	
	Hopper loader	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Extruder	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Microwave preheating system	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Deshumidifier	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Injectiong moulding machine	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U

Table 112. Dataset used for WP5 – MIX1.

	WP5	ECOINVENT
Wood composites production	**INPUT**	
	Bio-Polymer	Polyester-complexed starch biopolymer {GLO}| market for | APOS, U
	Wood	Wood chips, dry, measured as dry mass {RER}| market for | APOS, U
	OUTPUT	
	Wood composite	Wood composite MIX1
	WASTE	
	Offcuts WC1	Polyester-complexed starch biopolymer {GLO}| market for | APOS, U
		Wood chips, dry, measured as dry mass {RER}| market for | APOS, U
	EMISSIONS	
	-	
	ENERGY REQUIREMENTS	
	Eirich Mixer	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Microwaves	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Extruder	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Kneader machine	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Compression moulding	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Machining	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U

Table 113. Dataset used for WP5 – MIX3.

	WP5	ECOINVENT
Wood composites production	**INPUT**	
	Bio-Polymer	Polyester-complexed starch biopolymer {GLO}| market for | APOS, U
	Wood	Wood chips, dry, measured as dry mass {RER}| market for | APOS, U
	Graphite	Graphite {GLO}| market for | APOS, U
	OUTPUT	
	Wood composite	Wood composite MIX3
	WASTE	
	Offcuts WC3	Polyester-complexed starch biopolymer {GLO}| market for | APOS, U
		Wood chips, dry, measured as dry mass {RER}| market for | APOS, U
		Graphite {GLO}| market for | APOS, U
	EMISSIONS	
	-	
	ENERGY REQUIREMENTS	
	Eirich Mixer	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Microwaves	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Extruder	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Kneader machine	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Compression moulding	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Machining	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U

Table 114. Dataset used for WP5 – current.

	WP5	ECOINVENT
Metallic composites production	**INPUT**	
	Copper alloy	Copper {RoW}| aluminium alloy production, Metallic Matrix Composite | APOS, U
	OUTPUT	
	Metal composite	Wood composites CURRENT
	WASTE	
	Offcuts (scraps)	Scrap steel {Europe without Switzerland}| market for scrap steel | APOS, U
	EMISSIONS	
	-	
	ENERGY REQUIREMENTS	
	Eirich Mixer	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Microwaves	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Extruder	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Kneader machine	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Compression moulding	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U
	Machining	Electricity, medium voltage {Europe without Switzerland}| market group for | APOS, U

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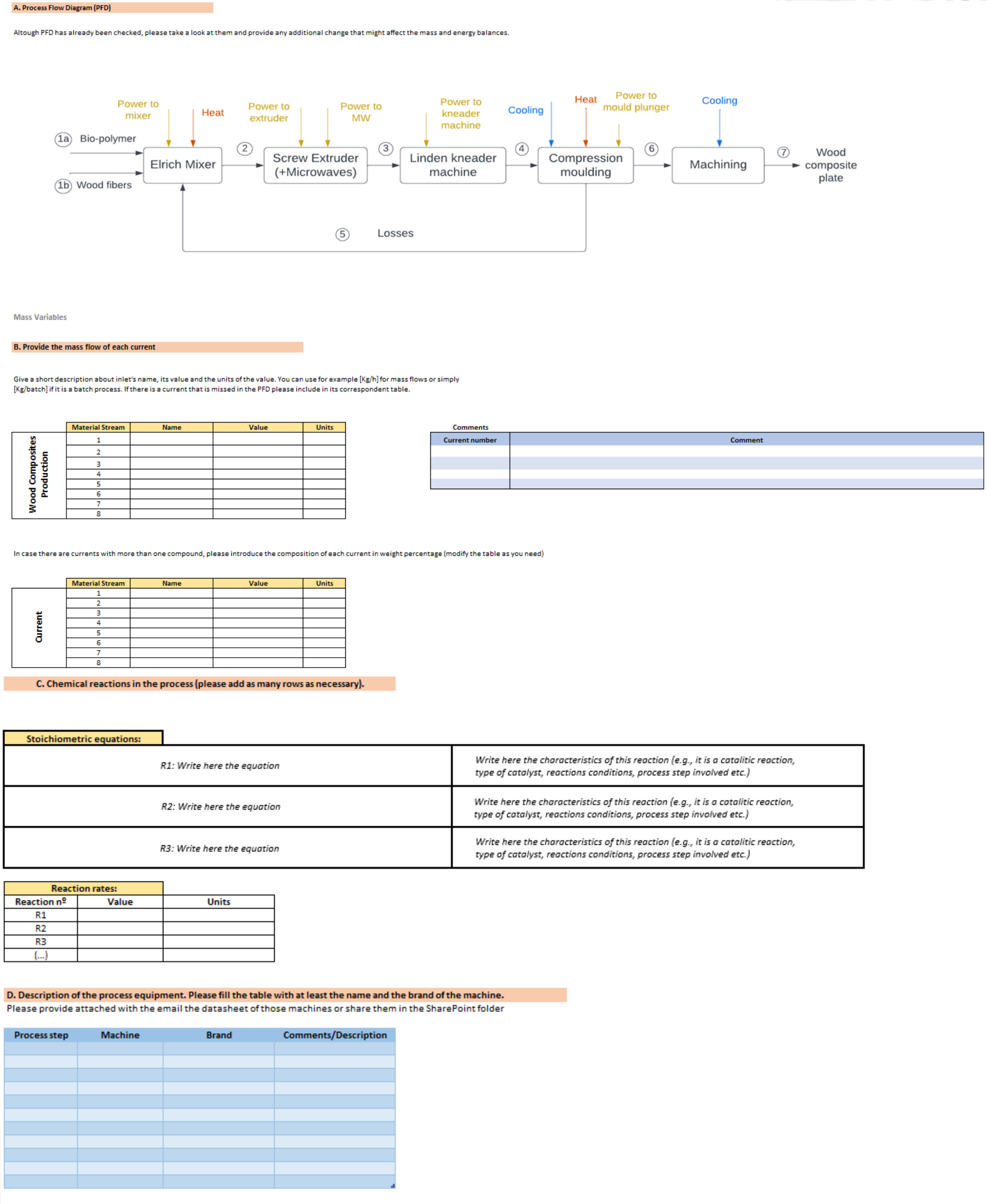
Annex 3: Questionnaires example



A. Process Flow Diagram (PFD)

Altough PFD has already been checked, please take a look at them and provide any additional change that might affect the mass and energy balances.

Mass Variables

B. Provide the mass flow of each current

Give a short description about inlet's name, its value and the units of the value. You can use for example [Kg/h] for mass flows or simply [Kg/batch] if it is a batch process. If there is a current that is missed in the PFD please include in its correspondent table.

	Material Stream	Name	Value	Units
Wood Composites Production	1			
	2			
	3			
	4			
	5			
	6			
	7			
	8			

Comments

Current number	Comment

In case there are currents with more than one compound, please introduce the composition of each current in weight percentage (modify the table as you need)

	Material Stream	Name	Value	Units
Current	1			
	2			
	3			
	4			
	5			
	6			
	7			
	8			

C. Chemical reactions in the process (please add as many rows as necessary).

Stoichiometric equations:

R1: Write here the equation	*Write here the characteristics of this reaction (e.g., it is a catalitic reaction, type of catalyst, reactions conditions, process step involved etc.)*
R2: Write here the equation	*Write here the characteristics of this reaction (e.g., it is a catalitic reaction, type of catalyst, reactions conditions, process step involved etc.)*
R3: Write here the equation	*Write here the characteristics of this reaction (e.g., it is a catalitic reaction, type of catalyst, reactions conditions, process step involved etc.)*

Reaction rates:

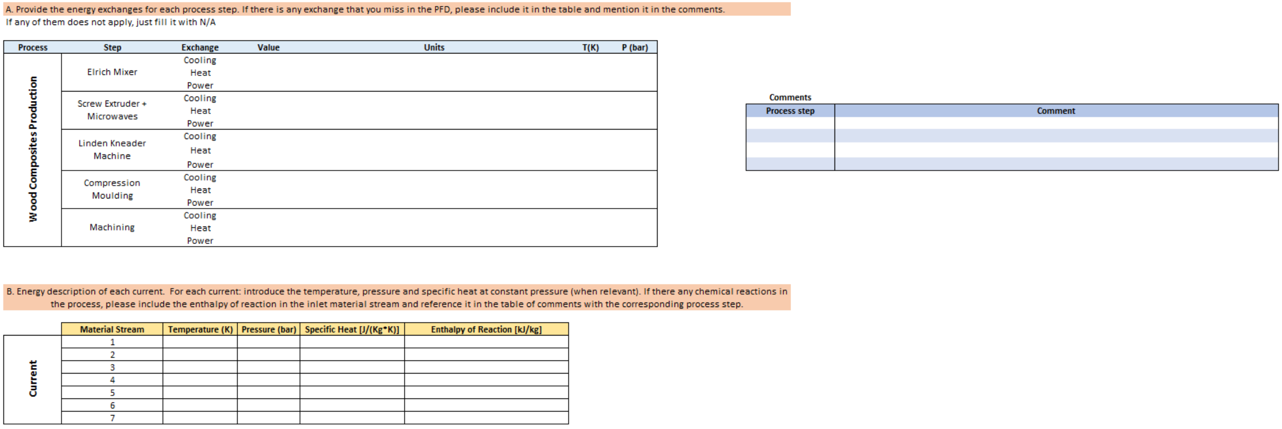
Reaction nº	Value	Units
R1		
R2		
R3		
(...)		

D. Description of the process equipment. Please fill the table with at least the name and the brand of the machine.

Please provide attached with the email the datasheet of those machines or share them in the SharePoint folder

Process step	Machine	Brand	Comments/Description

Figure 66. Example mass questionnaire for mass data.



A. Provide the energy exchanges for each process step. If there is any exchange that you miss in the PFD, please include it in the table and mention it in the comments.
If any of them does not apply, just fill it with N/A

Process	Step	Exchange	Value	Units	T(K)	P (bar)
Wood Composites Production	Elrich Mixer	Cooling				
		Heat				
		Power				
	Screw Extruder + Microwaves	Cooling				
		Heat				
		Power				
	Linden Kneader Machine	Cooling				
		Heat				
		Power				
	Compression Moulding	Cooling				
		Heat				
		Power				
	Machining	Cooling				
		Heat				
		Power				

Comments

Process step	Comment

B. Energy description of each current. For each current: introduce the temperature, pressure and specific heat at constant pressure (when relevant). If there any chemical reactions in the process, please include the enthalpy of reaction in the inlet material stream and reference it in the table of comments with the corresponding process step.

	Material Stream	Temperature (K)	Pressure (bar)	Specific Heat [J/(Kg*K)]	Enthalpy of Reaction [kJ/kg]
Current	1				
	2				
	3				
	4				
	5				
	6				
	7				

Figure 67. Example mass questionnaire for energy data.