

D3.3 Dataset with upscaling factors

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LIST OF ACRONYMS

LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
PFD	Process Flow Diagram

PROJECT INFORMATION

Project full title: Harmonised Life Cycle Assessment methods for sustainable and circular BIO based systems

Acronym: LCA4BIO

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6	BIOECONOMY FOR CHANGE	B4C
7	BUSINESS E-INCUBATOR GO-UP	GOUP
8	FUNDACION CENTRO DE SERVICIOS Y PROMOCION FORESTAL Y DE SU INDUSTRIA DE CASTILLA Y LEON	CESEFOR
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DELIVERABLE DETAILS

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Document Title:	Dataset of upscaling factors
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Abstract:	This document completes D3.2 to help building a proper Flow Process Diagram of the studied bio-based system. The main unit operations of bio-based systems are presented in six tables. Each table contains the main principles, type of equation and parameters needed to model diverse unit operations depending on their function.

Version	Date	Description
1.0	22.07.2025	Dataset with upscaling factors
2.0	24.07.2025	Revision of the document

DESCRIPTION

This document accompanies D3.2. and focuses on the different factors for scaling-up unit operations. The proposed methodology implies the use of simulation software to calculate the inventory by providing, at the same time, the technical assessment of the production chain. Bio-based systems generally follow a train of unit operations with four main parts: pretreatment, conversion, separation, product conditioning and utilities (Figure 1). The full description of Figure 1 is presented in D3.2.

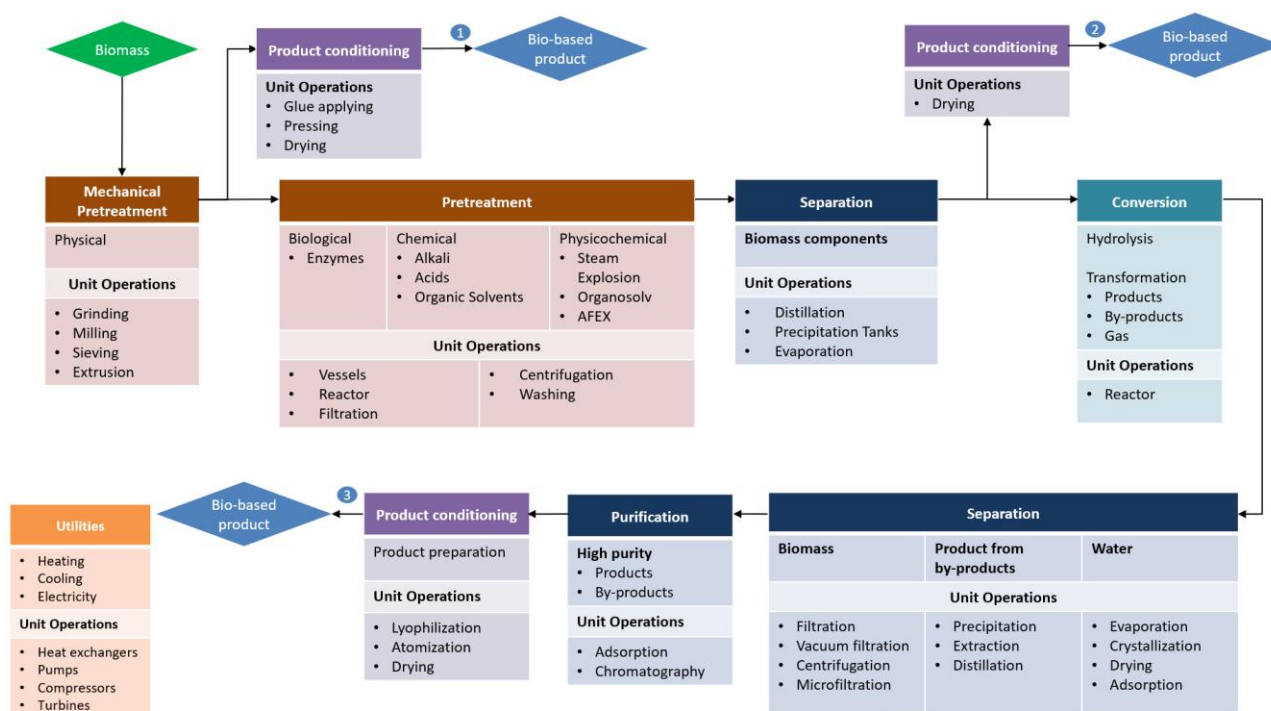


Figure 1. General flowsheet diagram of Bio-based Systems (BbS) including the most used unit operations for the production chain.

Simulation software provides mass and energy balances calculated upon chemical engineering principles. This software is accurate for chemical processes, especially when dealing with liquid and gas phase operations. However, for solid-liquid materials, it is quite a challenge, and several assumptions and calculations must be included. Diverse unit operations depending on their functionality are presented in the following Tables in order to guide the calculation of unit operation and their equivalent at high-TRL. Each unit operation depends on several parameters required to model it and to provide its corresponding material and energy flows that will be further used to build the Life Cycle Inventory.

Six tables are here presented depending on the function of different unit operations: 1) Size reduction, 2) solids separations; 3) liquid and gas separations; 4) heat exchangers; 5) vessel operations; and 6) transportation of fluids.

This is an intermediate version; several parameters and factors will be further detailed in the final version.

Table 1. Size reduction operations at High TRL

Unit Operation	Material Flow Inventory estimation	Energy Flow Inventory estimation	Scale / capacity	Uncertainty	Other considerations
Industrial shredder	NA (smaller particle size)	Calculation of power [1] * Torque * Rotational speed of the torque shaft * Maximum load	Depends on desired particle size For low load ~ 7.5 kW Mass flow rate of 5 ton/h ~132 kW		Rotation (Torque) speed that can impact the energy consumption, higher rotation requires high power
Grinders	NA (smaller particle size)	Calculation of power [2]: * Pressure * Volumetric flowrate * Efficiency	Efficiency ~ 30%		Equivalent at low-TRL: Mill and grinders
Vibratory Sieving	NA (smaller particle size)	Calculation of power [3]: * Mass * Velocity from rotations per minute and radius of the pulley * Efficiency	Depends on particle size	* Radius of pulley * Efficiency	Equivalent at low-TRL: Sieve shakers

NA: Not Applicable

Table 2. Solid/Liquid & Solid/Gas separation Units at High TRL

Unit Operation	Material Flow Inventory estimation	Energy Flow Inventory estimation	Scale / capacity	Uncertainty	Other considerations
Drying	<u>Principles:</u> * Activity coefficient models * Solid rate calculation at 25°C * No thermodynamic equilibrium calculation <u>Design parameters:</u> * Initial humidity * Final humidity * Air mass flowrate	Thermodynamic calculation of dew point for primary gas out stream Calculation of Power [4] * Evaporation percentages * Temperature * Enthalpies of hot air and ambient air	Lab scale: Drying column	* Efficiency	Equivalent at low-TRL: Oven or exposition to ambient temperature Similar equation for spray drying, drum drying and rotatory [5]
Filtration - Press - Depth	<u>Design parameters:</u> * Cake moisture * Suspended Solids in liquid phase	Calculation of power <u>Design parameters:</u> * Flowrate via Darcy equation * Ergun equation for pressure drop (ΔP) across a packed bed or filter media. * Efficiency	Lab scale: Centrifuge Paper filter	* Efficiency	For different kinds of filtration there is other parameters to take into consideration: Depth filtration: * Same flux (Q) * Same pressure drops (ΔP)
Centrifuge	Large or dense particles are concentrated in the cake while fine particles remain in the concentrate (liquid phase) <u>Design parameters:</u> * Pressure * Solid fraction in the overflow * Solid fraction in the underflow	Calculation of Power [6] Design parameters: * Operating speed (rpm) * Density * Volumetric flowrate * Efficiency	Efficiency ~ 30% 0 – 26 m ³ /h	* Separation of each component * Losses due to mechanical and electrical power	The maximum throughput for an efficient use of a centrifuge depends on the limiting sedimentation velocity (Navier Stokes' law) and the sigma factor.
Membrane filtration - Micro (0.1 – 10 µm) - Ultra (1 – 100 nm) - Nano (<300 Da)	Separation of fine particles to obtain retentate and permeate <u>Design parameters:</u> * Selectivity * Permeability * Cut-off threshold (pressure) * Pore size * Permeation Flux (L/h.m ²) * Membrane's surface	Calculation of power [7]: * Transmembrane pressure	Based on membrane's surface	* Permeation Flux	

NA: Not Applicable

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Table 3. Unit operations for separation

Unit Operation	Material Flow Inventory estimation	Energy Flow Inventory estimation	Scale / capacity	Uncertainty	Other considerations
Liquid-liquid Extraction	Multi-stage unit operation <u>Principles:</u> * Liquid-liquid equilibrium, * Activity coefficient models for non-ideal solutions * Theoretical plates (N) <u>Design Parameters:</u> * Purity and recovery specifications * Number of theoretical plates (N) * Partition coefficient * Solvent * Contact time	Calculation of Heating/cooling energy: * Cooling or heating (depending on solubility of the liquid use for extraction) <u>Design Parameters:</u> * Constant temperature		* Non-ideal solutions * Scale factor * Solvent selection	* It is very selective * Easily scalable * Solvent recovery by other unit operations: distillation or evaporation [8] [9]
Absorption	Multi-stage unit operation [10] <u>Principles:</u> * Phase equilibrium (liquid/vapor) * Activity coefficient models for non-ideal solutions * Height equivalent to theoretical plates (HETP) * Liquid stream on top * Vapor stream from bottom <u>Design Parameters:</u> * Number of theoretical plates (N) * Pressure * Pressure drop * Efficiency of plates	Calculation of heating energy: (If required) * Thermodynamic calculation of output temperature <u>Design Parameters:</u> * Overhead molar flowrate * Heating in reboiler (kettle)		* Pressure drop * Separation Efficiency of plates	* Solvent recovery by other unit operations: distillation or evaporation
Distillation / Stripper	Multi-stage unit operation for liquid or vapor input streams [10] <u>Principles:</u> * Liquid-vapor equilibrium, * Activity coefficient models for non-ideal solutions * Height equivalent to theoretical plates (HETP) * Chemical reactions handled in liquid phase	Calculation of energy needs * Thermodynamic equilibrium for the calculation of the temperature at the top and bottom streams * Cooling in condenser * Heating in reboiler (kettle) <u>Design Parameters:</u>		* Non-ideal solutions * Heat loss	Specific calculations with constraints on recovery rate can be possible for its design

	<u>Design Parameters:</u> * Number of theoretical plates (N) * Feeding plate(s) * Sampling plate(s) * Reflux ratio * Distillate flowrate	* Reflux ratio * Distillate flowrate			
Decanter	<u>Principles :</u> [10] * Liquid-liquid equilibrium, * Activity coefficient models for non-ideal solutions <u>Design Parameters:</u> * Temperature * Pressure	Calculation of cooling		* Non-ideal solutions	
Membrane for gas separation	Thermodynamic equilibrium model Design parameters: * Membrane surface and length * Membrane thickness * Temperature * Transmembrane pressure * Permeabilities of compounds * Pressure drop	Calculation of power - Depends on transmembrane pressure change. (Power calculated from compressors reaching the desired pressure)		Membrane surface	

NA: Not Applicable

Table 4. Heating operations

Unit Operation	Material Flow Inventory estimation	Energy Flow Inventory estimation	Scale / capacity	Uncertainty	Other considerations
Heat-exchanger • Tubular • Flat plate • Crossflow	NA	<u>Design parameters</u> [10] * Fluid's flowrate * Fluid's enthalpy * Heat exchanger efficiency (η) <u>Modes of calculation</u> * Output temperature * Temperature difference (input/output) * Required heat exchange surface (A) and Global coefficient of heat transfer (U)	Tubular : $\eta = 70\%$ Flat plate : $\eta = 90\%$ Crossflow : $\eta = 75 - 85\%$ [11]		
Evaporator/Condenser	<u>Design parameters:</u> * Pressure (constant) <u>Principles</u> * Liquid-vapor saturated properties	Latent heat of phase change			
Boiler	<u>Design parameters:</u> * Pressure (constant) <u>Principles</u> * Liquid-vapor saturated properties	Latent heat of phase change			

NA: Not Applicable

Table 5. Vessel operations

Unit Operation	Material Flow Inventory estimation	Energy Flow Inventory estimation	Scale / capacity	Source of Uncertainty	Other considerations
Stirring tanks	<u>Design parameters:</u> * Working volume, * Ideal mixing	Calculation of Stirring power: $E(kW) = \rho \cdot N_p \cdot N^3 \cdot D_A^5$ With N: agitator Rotation speed (rpm) N _p : Impeller Flow number ρ : Mixture density (Kg/L) $D_A \text{ Agitator diameter (m)} : \frac{1}{3} \left(\frac{4}{3} \cdot \frac{V_{reactor}}{\pi} \right)$	Depending on working volume	* Impeller flow number	Rotation speed at low-TRL is not equivalent at high-TRL
Stirring Reactors	<u>Design parameters:</u> * Working volume, * Residence time. <u>Reactions:</u> * Kinetic equations * Stoichiometric yields	Calculation of Stirring power * Same as stirring tanks Calculation of heating energy: * Estimation of thermal requirement to reach the reaction temperature, * Heat of reaction from thermochemical properties of components (enthalpy of formation) * Adiabatic or constant temperature operation * Heat loss	100 L – 10 m ³ [12]	* Heat loss to wall * Reactions in gas or liquid media * Thermodynamic model * Variable Stoichiometric yields	Equivalent at low-TRL: Erlen
Plug Flow Reactors	<u>Design parameters:</u> * Vessel volume, * Demand on liquid volume by the operation is divided by the operation's working to vessel ratio * Characteristics of the reactor: - Length - Internal diameter - External diameter <u>Reactions:</u> * Kinetic equations	Calculation of heating energy: * Estimation of thermal requirement to reach the reaction temperature <u>Design parameters:</u> * Temperature profile can be fixed * Temperature of the wall * Assumption of adiabatic operation		* Reaction kinetics * Heat loss to wall	Hydrodynamics can be considered. Conversion can be enhanced by increasing the length of the reactor
Bubble column reactors	<u>Design parameters:</u> * Volume and design pressure <u>Reactions:</u> * Kinetic equations * Stoichiometric Yields	No energy for stirring Calculation of Heating energy: * As for a Plug Flow Reactor			Large gas flow Easy to scale up
Settling tanks	<u>Design parameters:</u> * Solid and liquid components * Modeled as constituent separator	NA		Definition of components to split	

NA: Not Applicable

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Table 6. Equipment for transportation of fluids .

Equivalent at High TRL	Material Flow Inventory estimation	Energy Flow Inventory estimation	Scale / capacity	Source of Uncertainty	Other considerations
Pumps	NA <u>Design Parameters:</u> * Verify liquid phase stream	Calculation of power [13] <u>Design Parameters:</u> * Isoentropic efficiency: η * Pressure increase ΔP * Mass Flowrate	Based on efficiency curves	Efficiency at desired scale	Transport of liquid streams
Compressor	NA <u>Design Parameters:</u> * Verify gas phase stream	Calculation of power <u>Design Parameters:</u> * Isoentropic efficiency: η * Pressure increase ΔP * Mass flowrate	Based on efficiency curves	Efficiency at desired scale	Transport of gas streams
Turbine	NA <u>Design Parameters:</u> * Verify gas phase stream	Calculation of power <u>Design Parameters:</u> * Isoentropic efficiency: η * Pressure increase ΔP * Mass flowrate	Based on efficiency curves	Efficiency at desired scale	Used to recover energy in form of electricity

NA: Not Applicable

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