



CALiMERO

IMPROVING BIO-BASED INDUSTRIES LIFE CYCLE SUSTAINABILITY

D4.5 Report on the use of multi-objective optimization to optimize bio-based industrial processes

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PROJECT INFORMATION

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7	Luxembourg Institute of Science and Technology LIST
8	Technical University of Denmark DTU
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Abstract:	<p>This Deliverable (D) presents the final report of Work Package 4 in the CALIMERO project, which developed and validated a flexible Multi-Objective Optimization (MOO) framework for bio-based industrial process simulations within a broader sustainability viewpoint, including life cycle indicators from Life Cycle Assessment (LCA), Life Cycle Costing (LCC) and Social LCA (S-LCA) methodologies. Built in collaboration between academic and industrial partners, the framework has been integrated with process simulation models with LCA (e.g., via Brightway), apart from LCC and S-LCA to support comprehensive Life Cycle Sustainability Assessment studies. In addition, the MOO framework has been tested across five key bio-based sectors—woodworking, textile, construction, bio-chemical, and pulp & paper—through a series of demonstrators and case studies detailed in earlier documents (D4.1 to D4.3), including sensitivity and uncertainty analyses. This report summarizes the publicly shareable results and insights, highlighting the framework's real-world applicability and contribution to advancing a sustainable bioeconomy.</p>

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1 INTRODUCTION

This Deliverable (D) presents the final report for Work Package (WP) 4, which focuses on a Multi-Objective Optimization (MOO) framework for industrial process simulations, including life cycle sustainability indicators. As the culmination of WP4, it showcases how the developed framework can be applied in real-world industrial settings. Created in close collaboration with industry partners, the framework was designed to be flexible and adaptable, allowing to define and adjust key variables and objectives based on the specific needs of different industries.

The main goal of this D is to provide a public dissemination of the systematic, data-driven approach to optimizing bio-based industrial processes, while incorporating essential sustainability assessment tools. These include process simulation models, Life Cycle Assessment (LCA) calculation framework, Life Cycle Costing (LCC), and Social LCA (S-LCA), enabling a comprehensive evaluation of environmental, economic, and social impacts, covering Life Cycle Sustainability Assessment (LCSA) as a whole. The framework is particularly suited to five core bio-based sectors: Woodworking, textile, construction, bio-chemical, and pulp & paper, supporting their transition to a sustainable bioeconomy. This framework has been worked out in sensitive or confidential Ds with a first demonstrator in D4.1 (Simulation, LCA, LCC and MOO framework modules adapted to the specific needs of bio-based industrial sectors), an overview of approaches to integrate optimization with two concrete developed and applied approaches (a metaheuristic approach worked out by CTA, and a simplistic approach elaborated by LIST only applied to the textile case) in D4.2 (Development of links between simulation of industrial processes, LCA, LCC and MOO for bio-based industrial sectors), and an analysis of sensitivity and uncertainty through multiple runs of the simulation models in D4.3 (Validated simulation models with recommended solutions). This report concisely presents non-sensitive information and insights from these deliverables for the broad audience (see overview in [Figure 1](#)).

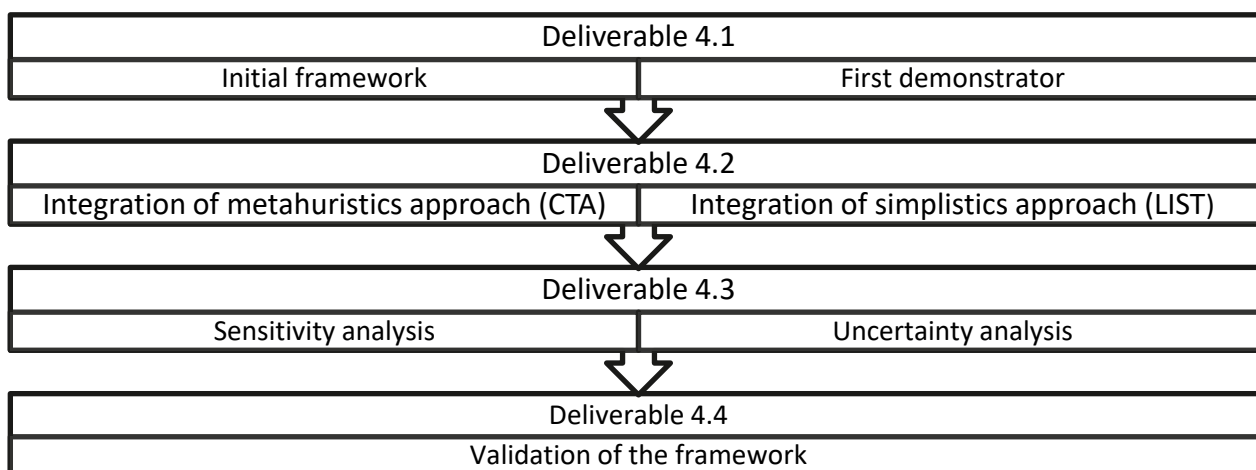


Figure 1. Overview of the associated deliverables which compose work package 4 of the CALIMERO project.

To verify its effectiveness, the framework was rigorously tested under D4.4 (MOO validated framework for bio-based industries), which played a key role in validating its real-world application. This validation involved applying the framework to specific simulation models, carrying out detailed case studies, and assessing practical industry scenarios. The results confirm that the framework is not only feasible and practical, but also provides valuable guidance for industries seeking to enhance sustainability, while balancing operational efficiency and economic viability.

2 BASICS OF MULTI-OBJECTIVE OPTIMIZATION OF PROCESSES TOWARDS OPTIMAL SUSTAINABILITY

2.1 Definition of key concepts and theoretical framework

2.1.1 Life cycle assessment methods

The LCSA module provides a comprehensive approach to evaluating the sustainability of industrial processes by integrating environmental, economic, and social factors. It combines LCA, LCC, and S-LCA methodologies to offer a well-rounded analysis. Beyond just assessing sustainability, LCSA also serves as a strategic tool that helps businesses incorporate sustainable practices into their operations, driven by evolving regulations and growing consumer expectations. By fostering innovation and improving operational efficiency, this approach supports the adoption of more sustainable industry practices. With a mix of quantitative and qualitative indicators, LCSA enables companies to make informed decisions that balance financial feasibility with environmental responsibility and social impact.

To implement LCA, among else the open-source Python library Brightway 2.5 was used, along with the biosphere3 and Ecoinvent 3.9.1 databases. This combination enables the systematic tracking of material and energy flows, as well as their associated environmental impacts. A comprehensive and reliable database is essential for capturing a wide range of environmental stressors across the product life cycle.

In LCA, inventory data alone (e.g., kilograms of CO₂ emitted) does not directly inform about environmental impacts. This is where Characterization Factors (CFs) play a key role. CFs convert inventory flows (e.g., emissions or resource use) into potential environmental impacts, such as global warming or human toxicity by applying scientifically derived multipliers. To improve the accuracy and completeness of impact assessments, new toxicity CFs were integrated, and missing elementary flows were added to the Environmental Footprint (EF) method template. These enhancements strengthened the methodological robustness and reliability of the results. Moreover, a limited hotspot analysis methodology was used—hotspot analysis calculations are shown in D4.1—with functions to calculate the most relevant impact categories.

In accordance with the consortium agreement, the assessment focused on economic performance alongside environmental evaluation, enabling a multidimensional view of sustainability. The economic analysis was conducted through LCC, with particular emphasis on key financial indicators: Levelized Cost of Production (LCOP), Net Present Value (NPV), and Operational Expenditures (OPEX). Among these, OPEX was selected as the primary optimization criterion, as it plays a decisive role in assessing long-term financial feasibility, especially in sectors with high recurring operational costs, where reducing OPEX can significantly improve overall economic sustainability.

Dedicated modules were developed for calculating both the LCOP and the Job Creation Potential (JCP) within the textile case study, serving as a practical example of how S-LCA can be integrated with other sustainability assessments. In accordance with the S-LCA framework, JCP is identified as a mandatory socio-economic indicator to be optimized, reflecting the potential of a process or product to generate employment throughout its life cycle (Lefevre et al., 2019).

2.1.2 Process simulation model

When developing a simulation model for a specific process or product, different approaches can be used depending on the case studies defined in D2.2 (Identification and implementation of appropriate modeling strategy). One common method is the results-based approach, where simulation outcomes are analyzed to optimize processes by adjusting input parameters. Another method is the model-based approach, which either directly integrates a detailed simulation model or creates a simplified “surrogate model” that maintains accuracy while reducing computational complexity. A key advantage of using a surrogate model is its ability to run

multiple simulations efficiently, generating additional insights that support the results-based approach. By combining these strategies, the extracted simulation module helps identify key parameters that optimize product or process life cycles, ultimately reducing inefficiencies across the five bio-sector industries.

To ensure that each sector's simulation model accurately represents real-world conditions, we have applied various methodologies outlined in D4.2. These techniques are carefully selected to align with each industry's unique requirements, ensuring that the models are both robust and reliable. The accuracy of these simulations is validated through extensive sensitivity and uncertainty analyses, which help assess how variations in input data impact overall results. These validation steps not only identify potential inconsistencies, but also ensure that all significant parameters are properly accounted for, increasing confidence in the model's predictive capabilities.

For uncertainty analysis, we use the Monte Carlo method, which evaluates a broad range of possible outcomes by running multiple simulations with different input variations. This technique is integrated into a structured workflow to ensure systematic input sampling and meaningful interpretation of results. Additionally, for sensitivity analysis, we apply derivative-based Global Sensitivity Analysis (GSA) (Iooss & Lemaitre, 2015; Lacirignola et al., 2017; Saltelli et al., 2008) methods and the Sobol method (Sobol', 1990). These techniques measure how much each parameter influences overall model variability, allowing us to identify the most critical factors. By combining these advanced methods, we enhance the accuracy and reliability of our simulations, leading to more precise and insightful sustainability assessments.

2.1.3 Uncertainty Analysis

Several approaches exist to do uncertainty analysis. In WP4, a Monte Carlo-based method was used. According to Sin et al. (2009), Monte Carlo-based uncertainty analysis involves four key steps:

1. **Defining input uncertainty:** Uncertainty arises from measurement errors in parameter estimation.
2. **Sampling:** Latin Hypercube Sampling (LHS) is used to efficiently explore the uncertainty space.
3. **Monte Carlo simulations:** Run simulated model multiple times to assess variability.
4. **Result analysis:** The output distribution is analyzed to evaluate uncertainty propagation.

A detailed description of the methodology is provided in D4.3.

2.1.4 Sensitivity Analysis

Once the uncertainty analysis quantifies the model output's variability due to uncertain inputs, a Sensitivity Analysis (SA) is performed to determine the relative contribution of each input to this variability. With Monte Carlo one can generate samples of the inputs X , and their corresponding outputs y . When y is a non-trivial combination of X_1, X_2, \dots, X_n , the Monte Carlo approach allows to build its probability distribution. It consists in artificially sampling values from the distributions of X_1, X_2, \dots, X_n and using this sample for estimating the shape and the parameter values of y (Heijungs, 2020).

With the Monte Carlo generated samples can be used to perform regression-based SA, using the generated inputs X and their corresponding outputs y to estimate the regression coefficients β from the expression:

$$y = b_0 + \beta X + \epsilon$$

Here, β represents the Standardized Regression Coefficients (SRCs), which are obtained by normalizing the regression coefficients with respect to input and output variances. SRC values range from -1 to 1, indicating the relative importance of each input variable in influencing the model output. The computational tool easy-GSA was used to conduct this analysis. A detailed description of the methodology is provided in (D4.3).

2.1.5 Multi-objective Optimization

Optimization aims at finding the best possible solution to a problem by finetuning different parameters to achieve a desired goal that is defined in the objective function. This could include, for instance, maximizing efficiency, minimizing costs, or improving overall performance. Optimization is widely applied across fields like engineering, economics, and sustainability to make systems more effective and resource efficient. Depending on the complexity of the problem, optimization techniques can be deterministic, using explicit mathematical expressions (like in linear programming), or stochastic, which rely on probabilistic methods (such as evolutionary algorithms) to navigate large, nonlinear, or unpredictable search spaces.

MOO takes this a step further by trading-off among multiple, often conflicting, goals at the same time. Unlike traditional optimization, which seeks a single best outcome, MOO focuses on finding a set of solutions that strike a balance between competing objectives—this is known as the Pareto front. A solution is considered *Pareto optimal* if improving one aspect would mean compromising another. This concept is particularly useful in real-world scenarios where factors like cost, efficiency, and environmental impact must be weighted together.

There are several ways to tackle MOO problems. One can divide roughly between two key approaches for optimization. First, there are metaheuristic approaches that look for the optimal solution by varying input parameter values in an iterative way, searching for the optimal solution. In this type, evolutionary algorithms, like Genetic Algorithms and NSGA-II, are popular because they can efficiently explore large solution spaces. These methods mimic natural selection, evolving a population of solutions over multiple iterations to refine results. Second key type are approaches based on programming, where it is the aim to mathematically solve or just characterize the system, and derive results from this. Such approaches include Pareto-based methods, which generate diverse sets of optimal solutions for decision-makers to choose from. As already highlighted, a unique challenge for MOO is the way of considering multiple variables. This can be done by considering constraints and prioritization, leading to a set of (sub)optimal solutions. There are also scalarization techniques, which simplify multi-objective problems by converting them into a single-objective format using weighted sums or similar approaches (Böckler & Mutzel, 2015). This has been outlined in D4.2 and in the following sections.

2.1.5.1 Deterministic Mode

When optimization problems involve certain and fixed input data or system parameters, deterministic optimization methods are essential. In this case, it can be explicitly formulated the problem using mathematical models, typically involving objective functions and constraints. Mathematical programming is a class of precise optimization techniques used to find the best outcomes such as minimizing costs or maximizing profits—under a set of given constraints. It involves formulating a mathematical model in which the objective function defines the goal, and the constraints represent real-world limitations, like resource availability. The optimization process then consists of mathematically solving this model to determine the best solution.

Several key types of mathematical programming can be mentioned:

- **Linear Programming (LP):** In LP, both the objective function and the constraints are linear. This method is frequently applied to resource allocation problems, including production scheduling and transportation planning.
- **Integer Programming (IP):** A variant of LP, IP requires some or all decision variables to take on integer values. It is particularly useful for problems involving discrete choices, such as determining the optimal location for facilities.
- **Nonlinear Programming (NLP):** In NLP, either the objective function or at least one constraint is nonlinear. This approach is suited to more complex situations, such as optimizing energy systems or financial models, where linear assumptions are insufficient.
- **Mixed-Integer Programming (MIP):** MIP combines elements of LP and IP by allowing some variables

to be integers while others remain continuous. This hybrid structure enables the modeling of a broader range of real-world scenarios, such as supply chain design, scheduling, and logistics. Although more computationally demanding than pure LP—due to the combinatorial nature of integer variables—modern techniques like branch-and-bound and cutting-plane algorithms have significantly improved its solvability.

- **Quadratic Programming (QP):** QP is a special case of NLP where the objective function is quadratic (involving squared variables) and the constraints are linear. This formulation captures more complex relationships among variables, making it ideal for applications like portfolio optimization or cost functions with diminishing returns.

2.1.5.2 Stochastic

When optimization problems involve uncertainty in input data or system parameters, stochastic optimization methods are essential. Unlike deterministic optimization, which assumes that all inputs are known, and fixed, stochastic optimization explicitly accounts for uncertainty by incorporating probability distributions into the model.

There are two primary approaches to handling uncertainty in optimization:

- **Stochastic Programming (SP):** SP addresses uncertainty by modeling multiple potential scenarios, each associated with a specific probability. The objective is typically to find a solution that performs well on average or minimizes expected cost across all scenarios. This approach is widely applied in sectors like energy planning, financial portfolio management, and supply chain logistics, where future outcomes are inherently unpredictable.
- **Robust Optimization (RO):** RO takes a different approach by avoiding reliance on probabilistic data. Instead, it focuses on finding solutions that remain feasible and perform well under the **worst-case realizations** of uncertainty. This method is particularly useful when probability distributions are unknown or unreliable. RO emphasizes reliability and stability, ensuring that solutions maintain acceptable performance even in highly adverse conditions.

2.1.5.3 Optimization strategies & techniques

2.1.5.3.1 Ranking and selection methods

Ranking and Selection (R&S) methods are a class of statistical techniques used to identify the best-performing alternatives among a finite set of stochastic options. These methods are especially valuable when the performance of each alternative is uncertain and can only be estimated through simulation or sampling. The objective is to make a statistically reliable choice by allocating computational effort efficiently across alternatives.

Classic R&S procedures, such as the indifference-zone approach and Bayesian ranking, aim to balance the trade-off between the number of simulations and the confidence in selecting the best solution. These methods are often used in simulation optimization settings where analytical expressions for objective functions are unavailable or too complex. By providing confidence bounds on performance estimates, R&S techniques help mitigate the risk of selecting suboptimal solutions due to sampling noise.

R&S is commonly used in fields like manufacturing system design, healthcare resource planning, and service operations, where simulation models are prevalent and analytical optimization is not feasible.

2.1.5.3.2 Metaheuristic methods

While traditional stochastic optimization methods, such as stochastic programming, incorporate uncertainty directly into mathematical models with constraints, metaheuristic algorithms adopt a different strategy. Rather than explicitly modelling uncertainty, they use iterative search processes designed to efficiently explore complex solution spaces (Stork et al., 2022). These algorithms are particularly useful for solving highly nonlinear, multimodal, or non-polynomial (NP)-hard problems (Maheshwari, 2016), where classical methods struggle due to computational complexity or the nature of the solution space. Unlike exact methods, they do not guarantee finding the global optimum. Instead, they focus on finding good solutions in reasonable computational time, which makes them ideal for complex or high-dimensional problems. These methods are stochastic in nature, often using randomness to guide the search and avoid premature convergence to local optima. They are particularly useful in fields like engineering design, telecommunications, and machine learning where problem spaces are large and computationally expensive to explore exhaustively.

Some of the most prominent metaheuristic algorithms used in stochastic optimization are: Evolutionary Algorithms, Simulated Annealing Approaches, and Swarm Intelligence Algorithms. They will be briefly described in the following sections.

1. Evolutionary Algorithms

- **Genetic Algorithms (GA).** They are inspired by the process of natural selection and are a class of evolutionary algorithms that iteratively search for optimal solutions by simulating the process of evolution. The algorithm begins with an initial population of randomly generated solutions. It then applies selection, a process where the most promising solutions—those with the highest fitness—are chosen to pass their characteristics on to the next generation. These selected solutions undergo crossover, where pairs of solutions exchange portions of their parameters to produce new offspring. This mimics biological reproduction and allows the algorithm to explore new combinations of parameters.

To introduce variability and avoid premature convergence to local optima, mutation is applied. This step randomly alters one or more parameters in a solution, injecting diversity into the population and increasing the chances of discovering better solutions. By repeatedly applying these processes—selection, crossover, and mutation—the algorithm navigates a wide solution space. With each generation, the overall population "learns," gradually refining the process parameters. Over time, the algorithm converges on a set of solutions that represent optimal or near-optimal trade-offs among competing objectives, such as minimizing emissions while maximizing product yield or economic return.

- **NSGAI (Non-dominated Sorting Genetic Algorithm II).** NSGA-II is a popular variant of GA used for solving multi-objective optimization problems. It uses a fast non-dominated sorting approach and introduces concepts like elitism and crowding distance to maintain diversity in the population. NSGAI has been widely applied in engineering design, supply chain management, and network optimization (Deb et al., 2002).

2. Simulated Annealing Approaches

- **Simulated Annealing (SA).** It is inspired by the physical process of annealing in metallurgy, where a material is slowly cooled to remove defects and optimize its structure. In SA, a probabilistic approach is used to accept worse solutions early in the search to avoid getting trapped in local optima.
- **Adaptive Simulated Annealing (ASA).** It is an enhanced version of the traditional SA, which adapts the

cooling schedule dynamically based on the problem's characteristics. It is particularly effective for solving large-scale combinatorial optimization problems, such as scheduling, routing, and resource allocation.

3. Swarm Intelligence Algorithms

- **Particle Swarm Optimization (PSO)**. It is a population-based optimization technique inspired by the social behaviour of birds flocking or fish schooling. Each solution is represented as a particle, and particles move through the search space by following the current optimum particles.
- **Standard PSO 2006**. This variant of PSO incorporates inertia weights and constriction factors to balance exploration and exploitation. It's used in problems involving continuous optimization, such as parameter tuning in machine learning and function optimization.
- **Ant Colony Optimization (ACO)**. It is inspired by the foraging behaviour of ants, which leave pheromone trails to guide other ants to food sources. In optimization, artificial "ants" explore different solutions, and promising paths are reinforced with virtual pheromones.

2.1.6 Integrated framework

The diagram shown in [Figure 2](#) presents a computational approach to optimizing process parameters using Python-based simulations. This framework integrates process simulation, data transformation, and LCA techniques to evaluate key performance metrics. The entire system operates within an iterative loop, driven by a stochastic optimization algorithm that continuously refines process variables to achieve optimal outcomes.

At the core of this framework is the interaction between process simulation and LCA. The process simulation makes use of operational parameters of the studied system, which are then used by the Brightway Python package to parametrize the corresponding LCA and LCC models to obtain lifecycle-based impact indicators, making resort to so-called background data (describing the steps of the lifecycle that are located upstream or downstream the studied process across the entire value chain) available through existing Life Cycle Inventory (LCI) databases. The primary objective of this framework is to optimize process parameters in a way that enhances efficiency and sustainability. A customized evolutionary algorithm iteratively adjusts variables, reruns simulations, and reassesses results until the optimal configuration is identified. This structured approach ensures a balance between performance, economic viability, and environmental sustainability.

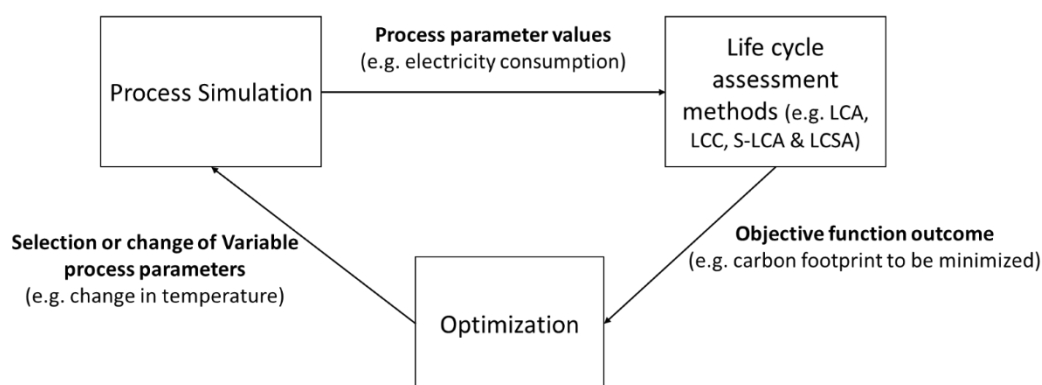


Figure 2. A high-level overview of the three modules of the optimization exercise and their main linkage (from D4.2).

The iterative feedback loop between process simulation and LCA allows for automated convergence to the optimal set of solutions, while considering environmental and economic performances consistently. This makes the framework a powerful decision-making tool for engineering and sustainability applications.

Before initiating LCSA, the optimization process begins by selecting key performance indicators and defining baseline scenarios. In sectors like woodworking, for example, optimizing the hot-pressing process—specifically adjusting temperature settings—enables a systematic evaluation of sustainability impacts. Establishing these benchmarks before simulation provides a reference point for assessing improvements post-simulation. This approach aligns with methodologies focused on LCC and sustainability performance (Li et al., 2016; Navarro et al., 2018). A simulation module for LCSA plays a critical role in enabling comprehensive evaluations of sustainability impacts across environmental, economic, and social dimensions. This integrated approach goes beyond traditional LCA by facilitating a more holistic understanding of sustainability performance. Through systematic simulations, interactions among different sustainability metrics can be analyzed, providing valuable insights for process optimization and strategic planning. For example, in the construction sector, LCSA simulations can assess the long-term performance of alternative materials and methods, supporting decisions that align with sustainability targets (Backes & Traverso, 2022; Li et al., 2016; Xu et al., 2017). Following LCSA simulations, the optimization module interprets the results and explores refinements to enhance sustainability outcomes. After optimizing temperature settings through simulation, uncertainty and SA are conducted. This step helps improve supply chain efficiency, minimize the carbon footprint, and address potential inaccuracies. Integrating Computational Trade-off Analysis (CTA) alongside LCSA simulations establishes a continuous improvement cycle, refining strategies and identifying opportunities for further sustainability enhancements. By incorporating uncertainty and SA, the optimization process ensures a well-balanced integration of economic, environmental, and social factors—leading to more informed and effective decision-making. These capabilities strengthen the robustness of decision-making by highlighting potential areas for improvement and refining strategies to maximize sustainability outcomes. This structured, simulation-based approach ensures balanced consideration of environmental, economic, and social factors, ultimately driving more resilient and informed engineering solutions.

3 DEVELOPED OPERATIONAL FRAMEWORKS

3.1 Integrated modelling with metaheuristic genetic optimization

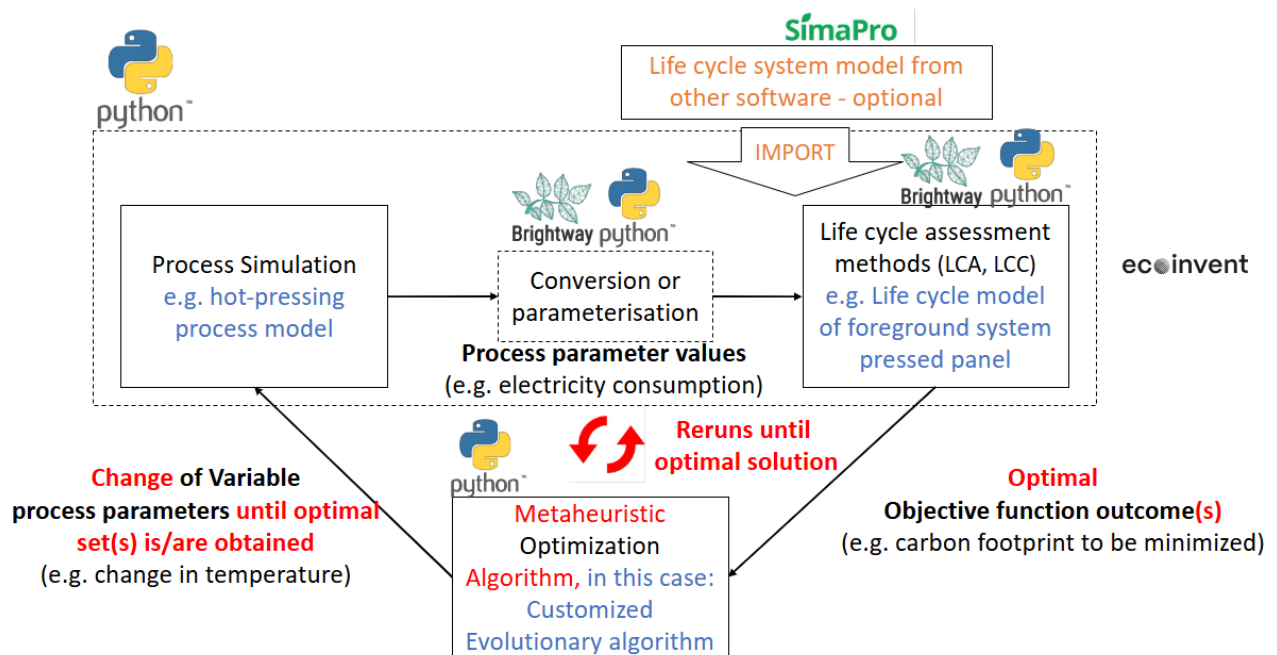


Figure 3. Overview of the applied approach of integrated modelling with metaheuristic optimization as developed by CTA, with specification of software environment, optimization algorithm (from D4.2).

CTA has developed a concrete optimization approach, applied notably to the woodworking hot-pressing case. However, the CTA framework is agnostic, i.e., any type of process model can be run, but the model should be available to be either run or called in the Python environment (see [Figure 3](#)). The following sections detail the methodology, with additional information available in D4.4.

3.1.1 Integration of process simulation

Developing a simulation module plays a crucial role in helping decision-makers assess the sustainability impacts of products and processes in a more comprehensive way. In fact, CTA by using this technique, creating a simulation model, helps decision makers to combine environmental, economic, and social assessments, providing a well-rounded perspective on sustainability. To do so, a parameterization module might be needed to transform process simulation parameters into life cycle inventory results. This can also be done within SimaPro software and then extracted to Brightway in a parameterized format. In any way a module in Python is obtained.

This integration highlights the importance of simulating interactions between these three dimensions, ensuring informed decision-making across various industries (Backes & Traverso, 2022; Li et al., 2016; Xu et al., 2017). Running LCSA simulations can also help pinpoint areas where resources are being used inefficiently and guide process optimizations toward sustainability goals. For example, as Backes and Traverso point out, the construction industry can benefit significantly from LCSA simulations by evaluating the long-term sustainability of different building materials and construction methods (Backes & Traverso, 2022). Hence, by incorporating simulation into LCSA frameworks, industries gain valuable insights into potential impact reductions and resource savings across multiple sustainability dimensions.

3.1.2 Integration of LCSA

The CTA framework is designed to be method-agnostic, allowing flexibility in integrating various tools and approaches. In practical implementation, however, the code has been specifically structured to work with Brightway 2.5 for modeling the foreground inventory system. Background data, including life cycle inventories and environmental flows, are sourced primarily from the Ecoinvent 3.9 and biosphere 3 databases, along with CFs for impact assessment methods.

This setup allows for comprehensive modeling of bio-based processes, ensuring consistency and reproducibility in sustainability assessments. In cases where the initial process modeling is conducted in other software, such as SimaPro, it is possible to extract and convert those models for integration into the Brightway environment, maintaining compatibility across platforms.

The modular nature of the framework enables seamless coupling with simulation tools, economic assessments, and optimization algorithms. This integration supports advanced decision-making through LCA, LCC, and MOO. The goal is to facilitate informed trade-offs between environmental, economic, and technical criteria. Further details can be found in D4.1.

3.1.3 Integration of Optimization

The optimization module within LCSA plays a key role in improving the effectiveness of sustainability analysis, both before and after simulations. It ensures that industrial processes are not only evaluated based on environmental, economic, and social factors but also refined to achieve the best possible outcomes across multiple objectives. By integrating optimization into the LCSA framework, industries can systematically explore and implement improvements that align with sustainability goals while maintaining efficiency in their operations.

To accomplish this, CTA used an evolutionary algorithm, a powerful stochastic optimization method inspired by natural selection. This algorithm iteratively improves a set of potential solutions by selecting the most promising

ones based on predefined sustainability criteria. Through processes like selection, crossover, and mutation, the algorithm navigates a vast range of possible solutions, continuously refining process parameters to achieve optimal trade-offs.

One of the biggest advantages of using an evolutionary approach in LCSA is its ability to balance conflicting sustainability objectives. In real-world scenarios, improving one factor—such as reducing carbon emissions—often comes at the expense of another, like increasing production costs. The evolutionary algorithm generates a Pareto-optimal front, a set of solutions that offer the best possible trade-offs between competing sustainability goals. This allows decision-makers to choose the most suitable option based on industry priorities, regulatory requirements, and market conditions.

To use this algorithm, CTA has overseen the development of a metaheuristic optimization framework in python, with at the core a tailored evolutionary optimization algorithm written in Python. This framework calls forth the life cycle method and process simulation model and runs it in an integrated manner for optimization. In other words, a linking is set up between these three modules in python code, where outputs of one serve as inputs for others, as shown in [Figure 3](#).

3.2 Enhanced process simulation with discrete linear optimization

LIST developed a more basic operational MOO approach where LCSA indicators (from LCA, LCC and S-LCA methodologies), were calculated and optimized. It has been applied to optimize the energy efficiency of a textile washing process, used as reference case study. The method relies on the use of LCSA indicators, e.g. calculated with the LCA software Activity Browser and Brightway, a package of Python, and through Excel templated created on purpose. Ecoinvent and PSILCA databases can provide the background information to the study for LCA and SLCA respectively. The optimization approach is discrete and linear and was proposed in a simplified way using Excel. In other words, life cycle impact scores (e.g. carbon footprint of electricity) were precalculated, e.g. from Activity Browser, and then multiplied with the process amounts, derived or directly obtained from the process simulation module in Excel. In case of derivation, this means that parametrization is applied and the flow values, e.g. dimensions of heat exchanger, are transformed into relevant process amounts, e.g., kg of steel needed, for which life cycle scores were obtained. [Figure 4](#) gives a schematic overview of the method applied.

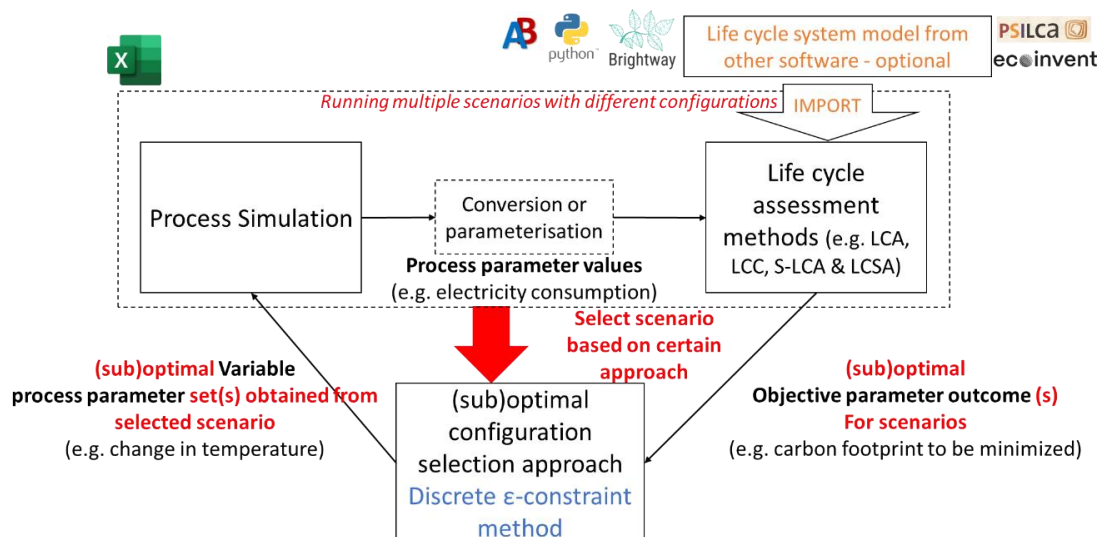


Figure 4. Overview of the applied optimization approach as developed by LIST, with specification of software environment, optimization algorithm (from D4.2).

3.2.1 Integration of process simulation

Creating a simulation module is essential for supporting decision-makers in evaluating the sustainability impacts of products and processes in a holistic manner. Leveraging this approach, LIST developed a simulation model for the specific case aimed at offering a user-friendly strategy to assist decision-makers in integrating environmental, economic, and social evaluations. This provides a more balanced and comprehensive view of sustainability performance. As mentioned earlier in our operational framework the process model is discretely run for many scenarios after operationalizing it, e.g. in excel as we did. For certain set of values in process parameters, discrete outcomes of technical characteristics and flow amounts can be obtained. For example, for a certain set of heat exchanger surface amounts, the heat demand and steel amount needed is obtained.

The integration underscores the value of modeling the interactions among the three sustainability pillars, enabling more informed choices across sectors. LCSA simulations also serve to identify inefficiencies in resource use and support targeted process improvements aligned with sustainability objectives. As a result, incorporating simulation into LCSA frameworks equips industries with actionable insights to drive reductions in impacts and optimize resource utilization across all sustainability dimensions.

3.2.2 Integration of LCSA

The operational framework developed by LIST (pre)calculates LCSA scores (e.g. using Brightway 2, typically in combination with its graphical interface, Activity Browser, or alternatively with SimaPro) for the foreground system or flows (e.g. the amount of the steel). Amounts for these flows are (indirectly) obtained from the process simulation model. The LCSA scores are then multiplied, i.e. implying linearity, with the latter amounts. To derive LCSA scores, foreground or background life cycle inventory data—such as inventories and environmental flows— can be drawn from databases such as the Ecoinvent 3.9 and biosphere 3 databases, complemented by CFs for impact assessment. For the social dimension (i.e., S-LCA), PSILCA can be used as the background database and can be accessed through any compatible software.

3.2.3 Integration of Optimization

While MOO often demands advanced, tailor-made algorithms due to its inherent complexity and the multitude of variables, a more straightforward method can be adequate or sufficient when the scope is limited, as is the case in the case study in textile bio-based sector (see [Section 4.2](#)), which involves only three parameters. In such situations, tools like Excel can be effectively used for the calculations, as was done in this integration. Given the narrow parameter space, viable solutions could be identified through simple optimization techniques and basic constraint management. Within this context, LIST applied a discrete ϵ -constrained method in an Excel environment. Despite the simplicity of the approach, the individual modules remain identifiable.

The method involves calculating the sustainability indicators across different scenarios, from which the (sub)optimal one(s) are identified. The term "(sub)optimization" is used to reflect the fact that scenario selection is based on a discrete set of predefined design alternatives, constrained by the technical limitations specific to the case study. As a result, the optimization process does not explore continuous variable ranges, and the technically optimal solution may lie outside the set of considered scenarios. Consequently, the approach follows a stepwise or discrete ϵ -constrained method. In practice, a hierarchy of life cycle impact indicators is established, and for each, a set of (sub)optimal parameter values are selected based on constraints and target outcomes. The viability of this method is highly case-dependent. Furthermore, Excel's data visualization capabilities allowed for effective analysis of trade-offs between competing objectives, making it a practical tool for small-scale optimizations that do not require sophisticated algorithmic approaches.

4 CASE STUDIES SET IN TARGET BIO-BASED SECTORS

Shifting toward a sustainable bioeconomy requires innovative strategies that optimize industrial processes while balancing environmental and economic trade-offs. Real-world case studies play a vital role in demonstrating how sustainability focused- optimization frameworks can be effectively applied. This section highlights case studies from key bio-based sectors, showcasing how multi-objective optimization and LCSA can enhance industrial performance.

The selected bio-based sectors—woodworking, textile, construction, bio-chemical, and pulp & paper—are industries with significant environmental impacts and substantial opportunities for sustainability improvements. Each sector faces distinct challenges, including resource efficiency, emission reduction, and process optimization. These case studies offer a comprehensive evaluation of sustainable industrial practices.

By applying the optimization framework described above across different industries, its adaptability and effectiveness are tested and validated. The results provide valuable insights into improving processes, reducing costs, and minimizing environmental impacts, helping decision-makers implement more sustainable and efficient production methods. These case studies serve as real-world examples of how industries can leverage data-driven strategies to align with circular economic principles, ultimately contributing to a more sustainable future.

4.1 Woodworking

This case study focuses on the hot-pressing stage in the production of Laminated Strand Lumber (LSL) boards made primarily from poplar wood. LSL is produced by drying wood strands, bonding them with adhesive, and compressing them under heat and pressure to achieve uniform density. After pressing, the boards continue to final processing. The hot-pressing section has been identified as a key area for improvement due to emissions released during press opening, which contain adhesive components and VOCs. These emissions are influenced by factors such as adhesive type, wood species, moisture content, and press conditions.

The objective is to develop and optimize a mathematical model to predict emissions based on operational variables. Data-driven models were created using MATLAB's Regression Learner, based on key parameters: pressing temperature, time, resin content, moisture content, and board density. Variables were scaled appropriately (see D2.2). The final models, which include an evaporation rate component, are implemented in Excel for practical use. After incorporating the case study into the framework, two alternative solutions (Solution 1 and Solution 2) are generated (see [Table 1](#)). Key process variables—pressing time, temperature, and adhesive concentration—are evaluated based on environmental impact categories such as climate change, human toxicity, and freshwater ecotoxicity, along with overall impact and OPEX. The results show that both alternative solutions outperform the reference case across all categories, demonstrating notable environmental and economic benefits.

Solution 2 achieves the greatest reduction in climate change impact (-8.71%), slightly outperforming Solution 1 (-8.59%). However, when it comes to human toxicity, Solution 1 shows a more significant improvement, reducing non-carcinogenic toxicity by -31.36% and carcinogenic toxicity by -38.38%, compared to Solution 2's reductions of -24.86% and -25.30%, respectively. A similar trend is observed in freshwater ecotoxicity, where Solution 1 achieves a -29.96% reduction, outperforming Solution 2's -20.91%. These findings suggest that Solution 1 is more effective in minimizing toxicity and environmental harm, making it the better choice for ecological and health-related concerns. From an economic perspective, both solutions contribute to lower operational costs. Solution 2 offers a slightly greater reduction in OPEX (-6.28%) compared to Solution 1 (-6.23%), making it the more cost-efficient option.

Table 1. Objectives results' from the solutions identified for the woodworking case study.

Objectives	Solution 1	Solution 2
Climate Change (kg CO ₂ eq.)	-8.59%	-8.71%
Human Toxicity: Non-Carcinogenic (CTUh)	-31.36%	-24.86%
Human Toxicity: Carcinogenic (CTUh)	-38.38%	-25.30%
Ecotoxicity: Freshwater (CTUe)	-29.96 %	-20.91%
Single score (Pt)	-8.41%	-8.50%
OPEX (€)	-6.23%	-6.28%

The selection between these solutions ultimately depends on the primary objective. If reducing human and ecotoxicity is the priority, Solution 1 is the better option. However, if cost savings and lower climate change impact are the main goals, Solution 2 is the preferable choice. Regardless of the decision, both alternatives represent a significant improvement over the reference case, supporting the shift toward more sustainable production practices.

To assess the impact of parameter estimation on emission predictions, an uncertainty analysis was conducted using a Monte Carlo simulation with 1,000 samples. For methanol (MeOH) emissions, the reference solution recorded the highest emissions with significant variability, whereas Solution 2 provided the most stable and precise predictions with the lowest standard deviation. Similarly, for acetic acid (HAc) emissions, the reference case exhibited the highest emissions, while Solution 2 demonstrated the least variability, reinforcing its robustness. However, for methylene diphenyl diisocyanate (MDI) emissions, Solution 2 consistently showed the highest emissions and variability under both uniform and normal air velocity distributions. Interestingly, emissions under normal distribution were slightly lower than those under uniform distribution, emphasizing the importance of air velocity assumptions in emissions modeling. These findings highlight the need for precise selection of model parameters and operational conditions to ensure accurate emission predictions.

An SA using the Standardized Regression Coefficient (SRC) method identified the most influential factors affecting emissions in different models. In the MeOH model, resin content had the strongest positive impact on emissions, followed by pressing time with a moderate effect. In the HAc model, pressing time was again the most significant factor, while pressing temperature had a moderate negative influence. For the MDI model, the Antoine Coefficient (C) and air velocity (U) were the key drivers of emissions, whereas other parameters like A and B had minimal impact. These findings show that emissions are highly sensitive to specific variables, highlighting the need for careful model validation and optimization to ensure accurate and reliable sustainability assessments.

4.2 Textile

In the textile case study, the focus was on analyzing the washing process of woven fabric after the desizing stage. This step aims to dissolve starch and other chemical substances that have impregnated the fabric during earlier processing. Since desizing involves the use of chemical agents to break down starch-based sizing materials, the subsequent washing is essential for removing the resulting maltose from the chemical reaction, along with any remaining wetting agents.

The process is carried out in a dedicated washing tank consisting of seven sections, where cold water is initially supplied. Since high temperatures are necessary to effectively dissolve and remove starch, heat is delivered through a closed-loop hot steam circuit integrated into the washing tank. The steam is generated by a gas boiler, which is shared with other processes within the facility.

The case study was initially evaluated by LIST using LCSA that consists of environmental, economic and social performances using, respectively, LCA, LCC and S-LCA. The analysis allowed to identify the hotspots of the

process, that resulted in the optimization opportunities. The whole assessments are available in deliverable D2.1.

The potential of improvement for such a case, as identified together with the industrial partner, lied in the waste heat energy valorization, as, after the washing process, originally the effluent water is sent to the wastewater treatment without any waste heat valorization. The installation of a heat exchanger would recover a share of the heat content of the wastewater before the discharge, allowing a reduction in the use of the boiler and a consequent direct decrement of fossil fuel combustion.

The goal of the optimization is to reduce the primary energy consumption provided by a gas boiler to supply the process heat, by integrating an appropriately sized heat exchanger into the process to harness heat recovery from the washing water. The novelty introduced by LIST in the optimization method lies in the strategy of the heat exchanger design, that is normally only based on technical-economic relations. In this case study, MOO method was applied to the design definition, including not only economic, but also environmental and social parameters. For this purpose, LCC, LCA and S-LCA were utilized. The concept is based on the relationship between the size of the heat exchanger and the boiler usage: the larger the heat exchanger, the more heat can be recovered, leading to a reduced reliance on the boiler. However, while a larger heat exchanger entails a higher initial investment, it also results in lower operating costs, as its operation requires no energy input. Nevertheless, the impact on other indicators is not immediately straightforward. Although the installation reduces gas combustion and thus brings environmental benefits, it also introduces new environmental costs associated with manufacturing the heat exchanger. Similarly, the social impacts related to managing the gas network must be weighed against those arising from the production of the heat exchanger.

Representative indicators were selected for each type of assessment. For the LCA, the 16 impact categories defined by the Environmental Footprint v3.1 method were calculated, weighted, and normalized to produce a single aggregated environmental score. For the economic evaluation, the LCC was calculated, incorporating all associated costs. Lastly, for the S-LCA, the JCP was used as the key indicator.

Several different scenarios were identified, each of them corresponding to a different size of the heat exchanger and, consequently, to a different percentage of use of the boiler. All three indicators were calculated for all the defined scenarios. The approach used was the discrete linear optimization, as described in [Section 3.2](#).

To determine the (sub)optimal scenario, the epsilon method was used. This technique sets acceptable ranges for each parameter, following a predefined order of priority, starting with the most influential factor. Through an iterative process, these ranges are gradually refined, progressively narrowing down the possible solutions until only one remains. In this case study, social impacts were prioritized first, followed by manufacturing costs, and then environmental impacts.

Once the optimal solution is identified, its performance is compared to a baseline scenario in which the washing process operates without any heat exchanger, relying solely on the boiler. Improvements are observed across all impact categories, as well as in operating costs, as shown in [Table 2](#). The most significant benefit is seen in the climate change category, with a reduction in kg CO₂ equivalents of 86.42%. The least improvement is noted in freshwater ecotoxicity, where the change remains below 10%, being in any case a good result. Overall, the average toxicity reduction is 32.83%. Operating costs decrease by almost 30%, but as the CAPEX of the new heat exchanger is huge, the LCC indicator increases of 42.73%. Another positive effect is detected on the Job Creation Potential, which increases by 12.38%.

After the identification of the optimal design alternative, the result was included in the simulation process of the full washing system (the washing process, and heat exchangers) that was performed using the software Aspen plus by DTU. In this analysis, further parameters may be altered besides the heat exchange surface area,

beyond what the industrial partner foresaw to alter.

Table 2. Objectives results' from the solutions identified for the textile case study.

Objectives	Solution
Climate Change (kg CO ₂ eq.)	-86.42%
Human Toxicity: Non-Carcinogenic (CTUh)	-32.09%
Human Toxicity: Carcinogenic (CTUh)	-58.26%
Ecotoxicity: Freshwater (CTUe)	-8.23%
Single score (Pt)	-67.26%
OPEX (€)	-28.98%
LCC	+42.73%
Job Creation Potential (JCP)	+12.38%

To assess the impact of uncertainties, an analysis was conducted by DTU on the overall heat transfer coefficient (U) and its influence on heat recovery and the required heat exchanger surface area (A). A Monte Carlo simulation using uniform and triangular distributions showed that the choice of distribution significantly affects the predictions. When U follows a normal distribution, the mean heat exchanger surface area (A) is the highest, with greater variability. In contrast, the triangular distribution yields lower mean values with less variation. These results emphasize the importance of careful statistical modeling, as even small fluctuations in the overall heat transfer coefficient (U) can lead to notable differences in system performance predictions.

The SA was performed by DTU using the software Aspen Plus. The SA aims at analyzing the three aspects that drive the energy efficiency of the case study, that are listed as i) split ratio of the valves of the pipes for the cold-water supply into washing tank; ii) flow rates and temperatures of the recycled streams; iii) the design specification of the heat exchanger. After running over 50,000 simulations, the analysis shows that the intermediate sections of the washing tanks are the most affected by changes in split ratios, that were made varying from 0 to 1 at 0.2 steps intervals. As split ratios below 0.5 yielded poor performance, the analysis narrowed its scope to split ratio between 0.5 and 1, with increments of 0.125, focusing only on sections 2 and 3 as more representative.

The following key results were highlighted:

- An increase in the split ratios is inversely proportional to the heat load on central sections of the washing tank.
- As the split ratio rises, the heat duty on the heat exchanger correspondingly increases.
- Despite the shifting heat loads, the total heat duty in the system remains relatively unchanged.

Afterwards, three operational scenarios were identified, defining different operations of the same process.

- Scenario 1: baseline operation without recycling process wastewater and without heat exchanger. All the sections of the tank have the split ratio equal to 0.
- Scenario 2: total wastewater recirculation from the washing tank, with the split ratio set to the maximum opening.
- Scenario 3: focusing on minimizing the use of steam and water utilities, it foresees the split ratio of all sections equal to 1, with the exception of tank 4, that is set a 0.333.

The examination of the results proves that scenario 3 offers the best improvements in both energy and water efficiency, guaranteeing a more efficient water allocation. The final model in Aspen Plus highlights that optimizing heat recovery and selectively distributing water are critical strategies for improving energy efficiency in the washing process under analysis.

4.3 Construction

This case study aims to optimize the formulation of cellulose-based insulation materials by minimizing Heat Release Rate (HRR) and Total Heat Release (THR). Various compositions are evaluated through experiments and simulations to understand how additives and fiber types affect fire resistance and thermal performance. The optimization balances fire safety, thermal efficiency, and cost-effectiveness. Predictive models using statistical regression and machine learning estimate HRR and THR based on material properties. Environmental factors such as carbon footprint and recyclability are also considered.

Matlab's stepwiselm function is used to build robust predictive models, selecting the most relevant variables through stepwise regression. This method enhances model accuracy and supports the development of sustainable, fire-safe insulation materials. After incorporating the construction case study into the framework by assessing different material formulations based on their THR, environmental impact, resource efficiency, and OPEX. The framework generates 7 alternative solutions.

The results from [Table 3](#) indicate that Solution 4 is the most energy-efficient option, as it has the lowest THR. However, Solution 1 strikes the best overall balance, excelling in most environmental and resource efficiency categories, despite having a slightly higher THR. On the other hand, Solutions 2 and 3 exhibit higher THR values, making them less desirable in terms of energy efficiency but potentially advantageous in other specific areas.

When cardboard (CB) is introduced into the material formulations, Solution 5 stands out for its low THR and strong environmental performance. However, its lower Single score and higher OPEX make it less efficient in terms of resource use. Solution 7 offers a well-balanced option, maintaining a good compromise between THR and environmental sustainability, whereas Solution 6, despite excelling in certain areas such as climate change, material and energy resources, and particulate matter formation, is hindered by its high MRI. These results highlight the inherent trade-offs between heat release, resource efficiency, and cost, emphasizing the need for a well-rounded approach when selecting the optimal material formulation.

Table 3. Objectives results' from the solutions identified for the construction case study.

Objectives	Solution 1	Solution 2	Solution 3	Solution 4	Solution 5	Solution 6	Solution 7
Climate Change (kg CO ₂ eq.)	-96%	-56%	-63%	-90%	-92%	-79%	-90%
Material Resources (kg Sb eq.)	-96%	-95%	-96%	-99%	-99%	-98%	-99%
Energy Resources (MJ)	-97%	-70%	-75%	-34%	-95%	-86%	-93%
Particulate Matter (disease inc.)	-98%	-79%	-82%	-95%	-96%	-90%	-95%
Single score (Pt)	-91%	-63%	-69%	-92%	-35%	-82%	-19%
OPEX (€)	38%	29%	31%	33%	44%	25%	42%

To account for variability, an uncertainty analysis using Monte Carlo simulations confirms that THR values fluctuate significantly depending on the chosen solution and the inclusion of CB. While CB reduces variability, confidence intervals indicate notable statistical differences between solutions, underscoring the importance of careful material selection.

Additionally, an SA shows that key parameters have a more stable influence when CB is included in the formulation. Without CB, parameter effects are highly variable, suggesting reduced model robustness. With CB, the influence of parameters becomes more predictable. These findings reinforce the necessity of tailoring material compositions to optimize thermal performance while ensuring accurate and reliable heat release

predictions.

4.4 Bio-chemical

This case study focuses on improving the reactor section of a second-generation bioethanol process, aimed at recovering bioethanol through an energy-efficient downstream configuration. The background model is based on a plant-wide simulation by Prunescu et al. (2017) for the Meliora plant, where ethanol is converted to polymer-grade ethylene using three adiabatic fixed-bed reactors at different temperatures, as described by Bisgaard et al. (2017). Ethylene is obtained with >99.9% purity.

A detailed process simulation is developed in Aspen Plus to model this reactor train. The system includes three adiabatic reactors (REACTOR1, REACTOR2, REACTOR3) and an intermediate heater. The feed enters at 25.0°C, is preheated, and undergoes exothermic dehydration reactions across the reactors. Mass and energy balances, reaction kinetics, and thermodynamic models are used to predict temperature profiles and energy demands. This approach supports optimization of the reactor sequence by simulating reaction behavior and energy flows without physical trials.

The framework evaluates five different solutions by analyzing temperature variations, reactor length, and overall environmental and operational performance. Each solution presents distinct characteristics, influencing material stability, energy efficiency, and sustainability (see [Table 4](#)). Notably, Solution 5 operates at the highest temperature in Reactor 1 (450°C), while Solution 2 runs at the lowest (405°C). In contrast, Reactor 2 reaches its highest temperature in Solution 2 (439°C), whereas Solutions 3 and 4 maintain the lowest temperature (424°C). The temperature in Reactor 3 remains relatively stable across all solutions, fluctuating only slightly between 400°C and 404°C, suggesting that this factor has minimal impact on process variability. Reactor length also varies across the solutions, with Solution 5 featuring the longest Length 1 (0.70m) but the shortest Length 2 and Length 3 (both 0.30m). These differences reflect design trade-offs between structural stability and material efficiency.

From an environmental perspective, Solution 5 emerges as the most sustainable option, showing the lowest climate change impact, non-carcinogenic human toxicity, and carcinogenic human toxicity. However, Solution 2 also performs well, particularly in reducing freshwater ecotoxicity and overall environmental impact, making it a strong competitor. In contrast, Solution 1 has the highest environmental footprint, including the greatest climate change impact and the highest freshwater ecotoxicity, making it the least favorable from a sustainability standpoint. Solutions 3 and 4 fall somewhere in between, each demonstrating a mix of advantages and trade-offs. Notably, Solution 3 has significantly high freshwater ecotoxicity, making it a less desirable choice for ecological sustainability. From an economic standpoint, OPEX remains fairly consistent across all solutions, with Solution 1 having the lowest costs, while Solutions 2 and 5 incur slightly higher expenses. However, since the cost differences are minimal, economic factors are not the primary drivers in the decision-making process.

Solution 5 stands out as the most environmentally responsible option, making it the best choice for sustainability-focused industrial applications. Solution 2 also offers compelling environmental advantages, particularly in reducing ecotoxicity and total environmental impact. On the other hand, Solution 1 ranks as the least sustainable, despite its slightly lower operational costs. Ultimately, the best solution depends on project priorities—whether the focus is on minimizing climate change impact, optimizing reactor efficiency, or balancing sustainability with operational costs.

Key output parameters including reactor duty, ethanol conversion, ethylene selectivity, and ethylene yield are evaluated in the uncertainty analysis under consideration of reactor length (L) and diameter (D). The study makes normal distributions assumptions for L and D; the latter has more effect on the outputs. While reactor length shows a modest correlation, Monte Carlo simulations revealed that reactor diameter greatly influences

all performance measures. Supported by scatter plot analysis, the results show that increasing reactor diameter improves performance by improving residence time and mixing efficiency, so stressing the need of optimizing reactor diameter for better reactor operation.

Table 4. Objectives results' obtained from the solutions identified for the bio-chemical case study.

Objectives	Solution 1	Solution 2	Solution 3	Solution 4	Solution 5
Climate Change (kg CO ₂ eq.)	-70%	-82%	-74%	-76%	-82%
Human Toxicity: Non-Carcinogenic (CTUh)	-15%	-60%	-29%	-38%	-61%
Human Toxicity: Carcinogenic (CTUh)	-15%	-52%	-26%	-33%	-55%
Ecotoxicity: Freshwater (CTUe)	-46%	-75%	-37%	-36%	-28%
Single score (Pt)	-76%	-86%	-79%	-81%	-86%
OPEX (€)	-30%	-27%	-30%	-27%	-27%

Reactor performance is investigated in the SA by the water/ethanol ratio. Increasing the water fraction in the feed reduces the net ethanol flow; but, a higher catalyst/ethanol ratio increases ethanol conversion, so peaking at a 0.3 water fraction. Nevertheless, the increased catalyst consumption makes this not the ideal state. Higher water fraction results in a decrease in conversion and selectivity with a constant ethanol flow since the shorter residence time and higher heat capacity encourage side events. From 99% to 97% the feed composition changes from an azeotropic mixture to a 1:1 ethanol-water mixture, thus ethanol yield somewhat declines overall.

4.5 Pulp & Paper

This case study evaluates the environmental impact of alternative chemical recovery routes in a pulp plant, aiming to reduce the EF of pulp, while maintaining sodium/sulfur balance. The focus is on electric plasma lime calcination (tend to lower bio and fossil fuel use), Lignin recovery (reduce recovery boiler load) and CO₂ capture from recovery boiler and calcination. The calcination section, identified as critical by the company, is prioritized for optimization due to its significant influence on plant efficiency and environmental impact.

A dynamic simulation model of the electric plasma lime calcination process is developed in Matlab/Simulink and Aspen. The model splits lime mud input between the ovens (traditional and electronic) and evaluates effects on flue gas emissions, and CO₂ capture, among other features. These insights help assess the environmental advantages of the alternative calcination route.

After setting up all the information in the framework, the analysis examines five different solutions based on the proportion of material fed into the electricity oven and their corresponding environmental and operational impacts. As the reliance on the electricity oven decreases from Solution 1 (100%) to Solution 5 (73%), there are noticeable shifts in climate change impact, human toxicity, ecotoxicity, and overall environmental performance.

Solution 1 records the lowest impacts in terms of human toxicity (both carcinogenic and non-carcinogenic) and climate change, although there are some impact categories higher in comparison with other evaluated solutions. On the other hand, Solution 5, which depends the least on the electricity oven, is the least effective in minimizing human toxicity and it has a slightly higher climate change impact. Solutions 4, 3, and 2 show a gradual improvement in environmental performance as the fraction directed to the electricity oven increases. In terms of economic performance, not remarkable changes are produced for OPEX between Solution 1 and Solution 5, so it can be said that economic factors do not play a role in decision-making. Instead, the choice should be driven by environmental priorities.

Moreover, the influence of varied combustion power contributions from different fuels (oil, saw dust, methanol, and gas) was also studied. The relative power contribution of the fuels varied in the specified ranges, keeping the total power constant. Compared with the default flows, which resulted in 1.087 (kg CO₂·kg CaO⁻¹), the CO₂ emissions increased to 1.151 when the pellets flow was highest, and it decreased to 1.053.

The use of an electric mesa oven could essentially reduce the emissions to zero given that the released CO₂ is captured for other purposes, e.g., lignin precipitation or electro-fuel. The CO₂ emissions are very dependent on the type of electricity. Electricity from coal power plants makes the emissions worse, while Swedish mix or wind/water electricity essentially reduces all emissions to renewable. The influence on CO₂ emissions of different fuel mixtures was low, in the order of 5%.

5 DISCUSSION

Case studies conducted across five bio-based sectors—woodworking, textile, construction, bio-chemical, and pulp & paper—demonstrate how MOO and LCSA enhance industrial sustainability. By integrating advanced computational tools, such as process simulations, LCA, LCC and S-LCA, the framework effectively identifies trade-offs and optimizes solutions tailored to each sector's unique challenges.

A key takeaway from all case studies is the intricate balance between economic and environmental factors. In the woodworking sectors, parameters such as pressing time, adhesive concentration, and heat recovery play a significant role in sustainability outcomes. Uncertainty and sensitivity analyses underscore the importance of selecting the right parameters to optimize emissions, energy consumption, and cost efficiency. For example, in the woodworking case study, Solution 1 minimized human and ecological toxicity, while Solution 2 achieved greater cost efficiency and lower climate change impact—highlighting the need to align objectives with industry priorities. For the textile case, it was also crucial to find a balance between the environmental and social, on the one hand, and economic results, on the other hand. A higher surface area for the heat exchanger area would unfavorably increase the LCC costs (although this is only for very high surface areas), but beneficially decrease the environmental impact and increase the JCP. Similarly, the Construction sector highlighted the trade-offs between THR, resource efficiency, and operational costs. Incorporating CB into material formulations improved stability and heat performance, demonstrating the importance of balancing material selection with sustainability goals. For the bio-chemical case study, it reinforced the impact of structural and thermal configurations on environmental and operational performance, with factors like temperature and reactor dimensions significantly influencing sustainability metrics. In the pulp & paper sector, the proportion of material fed into the electricity oven had a notable effect on environmental performance. Reducing oven reliance lowered toxicity and ecotoxicity but slightly increased climate change impact, illustrating the trade-off between greenhouse gas emissions and broader environmental concerns. These findings highlight the necessity of multi-objective decision-making, as no single solution universally outperforms others across all criteria.

From a methodological standpoint, the framework builds upon a robust combination of simulation, optimization, and decision-support tools to guide sustainability assessments. At its core, the CTA framework integrates evolutionary algorithms within the optimization module, allowing for an efficient exploration of complex, multi-dimensional solution spaces. Unlike conventional optimization techniques that may struggle with highly nonlinear and multi-objective problems, evolutionary algorithms iteratively refine solutions through mechanisms such as selection, crossover, and mutation, ensuring optimal trade-offs are identified. For the LIST framework, simplicity is key with a straight forward optimization approach, potentially used in Excel.

Additionally, the Monte Carlo simulation-based uncertainty analysis used to enhance result reliability by quantifying variations in key parameters. This statistical approach provides a probabilistic view of sustainability outcomes, ensuring that decision-makers account for uncertainties in material properties, emissions, and process efficiencies. On the other hand, SA complements this by identifying key drivers of sustainability

performance, allowing industries to prioritize adjustments that yield the most significant improvements.

Another key strength of the framework is its modular and adaptable structure, which ensures scalability across different industrial sectors. By seamlessly integrating LCA, LCC, and S-LCA, the framework enables a holistic evaluation of sustainability, bridging environmental, economic, and social dimensions. This modularity allows companies to customize the assessment process based on sector-specific challenges, making it a versatile tool for long-term strategic planning.

Ultimately, by combining advanced computational modeling, optimization algorithms, and robust statistical analysis, the framework provides a data-driven decision-making platform for industries aiming to enhance sustainability. This comprehensive approach not only supports regulatory compliance and sustainability reporting, but also fosters innovation by identifying cost-effective, resource-efficient, and environmentally responsible solutions.

6 MAIN CONCLUSIONS

The case studies underscore the transformative impact of MOO and LCSA in shaping a more sustainable industrial future. The developed framework has proven its adaptability across diverse bio-based sectors, successfully balancing economic viability, environmental responsibility, and operational efficiency—the critical pillars of sustainable production.

One of the key takeaways from this document is that sustainability-driven industrial optimization cannot rely on a one-size-fits-all approach. Each sector presents unique challenges, requiring tailored solutions that leverage data-driven insights to minimize trade-offs and maximize sustainability gains. By integrating process simulations, uncertainty and sensitivity analyses, and evolutionary algorithms, industries can make more informed, strategic decisions that optimize both economic and environmental performance.

Looking ahead, there is immense potential to further refine and enhance this framework. Incorporating real-time industrial data and machine learning could make optimization even more dynamic, allowing companies to adapt quickly to changing conditions and improve predictive accuracy. Additionally, expanding sustainability assessments beyond LCA to include S-LCA factors such as worker health, safety, and broader social implications would provide a more comprehensive and human-centered evaluation of industrial processes.

This report lays a strong foundation for integrating sustainability into industrial decision-making. By systematically fine-tuning process parameters and harnessing the power of advanced computational tools, industries can boost resilience, drive efficiency, and stay competitive in an evolving bioeconomy. More importantly, these insights serve as a practical guide for companies and decision makers striving to transition toward greener, more responsible production methods.

Ultimately, embracing intelligent optimization strategies is not just about improving current operations—it is about shaping a future where industries contribute to a thriving circular economy, minimizing their EF, and creating a more sustainable world for generations to come.

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