

Economic Feasibility Assessment of Bio-Based Vitrimers from Agrifood Residues: a Step Toward Sustainable Circular Economy

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The Cyclevit project, funded by Fondazione Cariplo, aims to develop innovative bio-based vitrimers—recyclable, self-healing polymers—using agricultural by-products (e.g., wheat straw, grape pomace, rice husk). A previous study discusses the use of combined autohydrolysis and organosolv treatments for recovering cellulose and lignin from agri-food waste more sustainably than traditional acid and alkaline hydrolysis. This work assesses the economic feasibility of producing bio-based vitrimers from agri-food residues using Monte Carlo simulations and a regression analysis, focusing on the minimum product selling price (MPSP). The average MPSP is €435.5 per kilogram, with potential reductions of 60% in best-case scenarios and increases of up to 400% in worst-case conditions. Key factors affecting MPSP include industrial performance metrics and raw material costs. The recycling design significantly reduces water consumption, aligning with green chemistry principles. However, the low technology readiness level (TRL) limits market competitiveness, highlighting the need for pilot-scale validation. Despite current economic challenges, bio-based vitrimers from agricultural residues demonstrates strong environmental benefits through enhanced resource efficiency and landfill diversion.

1. Introduction

The need to reduce reliance on fossil fuels has spurred research into renewable alternatives, such as converting agro-food residues into bio-based materials, food additives, energy, or high-value products (Tassinari et al., 2023). However, the shift to a circular bioeconomy faces challenges, including regulatory and societal pressures, as well as the economic and technical competitiveness of bio-based materials versus fossil-based ones (Molenveld and Bos, 2020). While fossil-based materials are cost-effective and perform well, they have major environmental downsides. The impact of bio-based materials varies depending on their feedstock, with agri-food residues being more sustainable than primary crops like maize (Hann et al., 2020). Although currently more expensive, bio-based materials are expected to become increasingly competitive as production scales up and technologies improve (Van Den Oever et al., 2017). In this context, the CYCLEVIT project, supported by Fondazione Cariplo, seeks to create innovative bio-based polymers called vitrimers, which are sourced from agricultural by-products. These materials merge the qualities of thermoplastics and thermosets, providing features such as recyclability, self-repair, and mechanical strength comparable to traditional plastics (Röttger et al., 2017). The raw materials of these polymers are lignin and cellulose, which can be sourced from agri-food residues such as wheat straw, grape pomace, and rice husks. Their utilization reduces the environmental impact of plastic production and mitigates waste disposal issues, contributing to more sustainable resource management. A previous study by Cipriani et al. (2024) investigated the combined treatments of autohydrolysis and organosolv for the recovery of cellulose and lignin from agri-food waste in a way that is more sustainable than the traditional process involving acid and alkaline hydrolysis, thereby reducing the need for highly polluting

chemicals. However, economic and technological challenges remain, particularly in terms of process scalability and industrial competitiveness compared to well-established fossil-based thermosets (Zhang et al., 2021). Within this framework, this study employs Monte Carlo simulations and a regression analysis to determine the minimum product selling price (MPSP) of the bio-based vitrimers produced from agro-food residues, thereby assessing the economic feasibility. Building on the scenarios provided by Cipriani et al. (2024), this work provides insights into cost optimization strategies and the critical economic factors affecting the scalability of bio-based vitrimers production. By evaluating the commercial viability of this process, the study establish a reference point for similar techno-economic analysis. The findings help identify potential pathways for cost reduction and highlight investment opportunities, thereby supporting informed decision-making in the development of sustainable bioeconomy pathways and emphasizing the importance of linking residue valorisation to economic performance.

2. Material and Methods

As previously stated, the purpose of this work is to assess the economic viability of recovering cellulose and lignin from wheat straw for the production of bio-based vitrimers. The production process was investigated in previous work by Cipriani et al. (2024) and summarized in Figure 1. Notably, Cipriani et al. (2024) investigated two different process configurations—one with acid liquor recycling or one without. The key difference lies in water consumption: recycling results in a saving of 83.51 L per kg of vitrimers produced. This design aligns with the principles of green chemistry and is more compatible with the sustainability goals of a circular bio-based production system. It reduces resource use, especially water, and lowers operating costs. Therefore, the economic analysis in this study focuses solely on this recycling scenario. Nonetheless, it is important to note that the need for enhanced water waste management infrastructure may lead to increased expenditures.

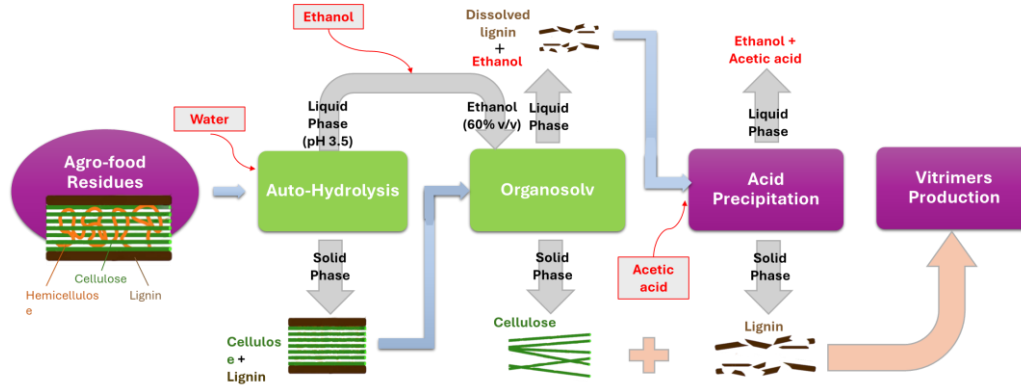


Figure 1 Fractionation process for cellulose and lignin recovery from residues for vitrimers production

2.1 Economic assessment

The economic evaluation of the process is based on an assessment of the MPSP. Given the low technology readiness level (TRL) and the uncertainty surrounding the production process, the MPSP represents the lowest price at which the product can be sold while ensuring non-negative profitability. This metric is critical for evaluating the economic feasibility and market potential of early-stage technologies, as it provides insight into their competitiveness relative to existing alternatives in terms of production costs. In this study, profitability is evaluated using the net present value (NPV) method. The MPSP is determined as the minimum price that achieves break-even profitability, i.e., when $NPV = 0$, as expressed by the following equation (Eq. 1),

$$NPV = -(1 - \alpha)I - A \left[\frac{(1 + r)^N - 1}{r(1 + r)^N} \right] + NB \left[\frac{(1 + r)^{\tau+1} - 1}{r(1 + r)^{\tau}} \right] - \beta I \left(\frac{1 + g}{r - g} \right) \left[1 - \left(\frac{1 + g}{1 + r} \right)^{\tau} \right] + \frac{\gamma I}{(1 + r)^{\tau}} \quad (1)$$

where: α , the portion of total capital investment (I) financed by debt with an interest rate ρ , paid for N years; A , the fixed annuity to pay the loan since the second year of the investment, computed as $A = \frac{\alpha I \rho}{1 - (1 + \rho)^{-N}}$; NB , the annual net benefit; r , a real discount rate; β , the maintenance cost, which is expressed as a percentage of the initial investment, expected to grow exponentially after the first year at an annual rate of g ; and γ , a share of the investment to include a salvage value at the end of the payback period τ . The NB is assumed to remain constant and equivalent (in nominal terms) to the estimated gross profit per year in the base year, which is equal to the difference between total revenue, generated solely from the sale of vitrimers (q), and variable costs (VC).

Given the low TRL of the laboratory experiment, the available information is limited to the material flows of inputs (i) and relative technological coefficients (ε_i). Therefore, once the unit input prices p_i were collected from various sources (see Table 1), the total variable cost was computed assuming a Leontief technology cost structure and a share (δ) of raw material cost in the average variable cost as

$$VC = \left(\sum \frac{p_i}{\varepsilon_i} \right) \frac{(1 - \delta)}{\delta} q \quad (2)$$

Based on the same principle, the total capital investment was estimated assuming a share (θ) of the variable cost in the average total cost as

$$FC = VC \frac{(1 - \theta)}{\theta} \quad (3)$$

By varying the parameters of δ and θ , it is possible to simulate different industrial settings, assuming higher or lower levels of raw material use and fixed costs within the production function. In general, a higher proportion of average fixed costs is more likely to represent conditions associated with smaller plant size. Table 1 summarizes all parameters used in the computation of the NPV and the estimation of the MPSP.

Table 1: Economic parameters for the MPSP computation.

Parameter	Name	Value	Unit	Source
δ	Share of raw materials costs	0.5	%	Assumed
θ	Share of variable costs	0.6	%	Assumed
Inputs prices	Wheat straw	0.070	EUR/kg	(ISMEA, 2023)
	Water	0.004	EUR/L	(Eurostat, 2023)
	Ethanol	1.060	EUR*/L	(Nandiyanto et al., 2022)
	Acetic acid	0.500	EUR*/L	(Alibaba, 2023b)
	Beneze diboronic acid	6.900	EUR*/kg	(Alibaba, 2023c)
	Thioglycerol	7.800	EUR*/kg	(Alibaba, 2023a)
	Epoxidized soybean oil	2.800	EUR*/kg	(Alibaba, 2023b)
α	Debt share of the investment	0.5	%	(Golberg et al., 2021)
ρ	Interest rate	0.05	%	(Golberg et al., 2021)
N	Loan duration	10	years	Assumed
r	Real discount rate	0.05	%	Assumed
γ	Salvage value share	0.05	%	Assumed
β	Maintenance cost share	0.005	%	(Golberg et al., 2021)
g	Annual growth rate of maintenance cost	0.005	%	(Golberg et al., 2021)
τ	Payback period	4	years	Assumed

Note: *Indicates US dollars converted at an exchange rate of 1 USD = 0.923 EUR (Exchangerates, 2023).

Given the uncertainty surrounding the low TRL and the underlying assumptions, an economic evaluation of the production process was performed using a broad set of scenarios generated through Monte Carlo simulations. A uniform distribution was applied to the parameters δ and θ , while a PERT distribution—assuming a $\pm 30\%$ range—was used for the remaining variables. The duration of the biomass supply and the loan repayment period were held constant. A total of 10'000 independent and random iterations were performed. To assess the relative influence of exogenous variables on MPSP variability, a log-log ordinary least squares (OLS) regression was then conducted, using MPSP as the dependent variable and all model input parameters as independent variables. The log-log specification allows for the interpretation of the estimated coefficients as elasticities.

3. Results and discussion

Descriptive statistics from the Monte Carlo simulations are presented in Table 2, summarizing the key parameters in the analysis. These include industry performance indicators, technology coefficients, input prices, and economic factors affecting the NPV of the investment. These statistics offer an overview of the stochastic nature of the modelled scenarios, enhancing understanding of system dynamics and supporting strategic decision-making for different industrial and investment contexts. Table 2 also reports the estimated MPSPs, averaging EUR 435.5 per kg for the final bio-based vitrimers. Consistent with previous studies, the selling price of bio-based vitrimers results prohibitively high (Bass and Epps, 2021). The MPSPs varies significantly across scenarios—decreasing by approximately 60% in the best case and increasing by up to 400% in the worst case—

resulting in a right-skewed distribution (Figure 2a). This skewness indicates elevated investment risk, as in half of the most unfavourable situations (beyond the mean), the price uncertainty is substantially higher.

Table 2 Descriptive statistics from the Monte Carlo simulations.

	Min.	1st Qu.	Median	Mean	3rd Qu.	Max.
<i>Industry performance</i>						
Share of raw materials costs	0.300	0.397	0.500	0.499	0.600	0.700
Share of variable costs	0.100	0.299	0.502	0.500	0.701	0.900
<i>Technological coefficients</i>						
Biomass	4.054	5.250	5.726	5.727	6.204	7.303
Water	169.90	214.90	235.20	235.00	255.10	302.70
Ethanol	31.55	40.56	44.32	44.32	48.09	57.28
Acetic acid	4.897	6.267	6.839	6.851	7.424	8.782
Benze diboronic acid	0.065	0.082	0.090	0.090	0.098	0.116
Thioglycerol	0.085	0.110	0.120	0.120	0.130	0.155
Epoxidized soybean oil	0.364	0.467	0.509	0.509	0.552	0.657
<i>Input prices</i>						
Biomass	0.050	0.064	0.070	0.070	0.076	0.090
Water	0.003	0.004	0.004	0.004	0.004	0.005
Ethanol	0.756	0.976	1.064	1.064	1.152	1.369
Acetic acid	0.356	0.457	0.500	0.500	0.542	0.648
Benze diboronic acid	4.959	6.321	6.896	6.899	7.484	8.908
Thioglycerol	5.609	7.154	7.789	7.799	8.457	10.008
Epoxidized soybean oil	2.007	2.562	2.802	2.799	3.034	3.608
<i>NPV economic factors</i>						
α	0.356	0.459	0.501	0.501	0.542	0.648
ρ	0.036	0.046	0.050	0.050	0.054	0.064
r	0.011	0.039	0.050	0.050	0.061	0.089
γ	0.035	0.046	0.050	0.050	0.054	0.064
β	0.004	0.005	0.005	0.005	0.005	0.006
g	0.004	0.005	0.005	0.005	0.005	0.006
τ	2.061	3.461	4.143	4.169	4.846	6.903
MPSP (EUR/kg)	170.50	308.40	392.90	435.50	516.00	1742.40

The current state of bio-based technology reveals a substantial cost gap compared to conventional fossil-based alternatives, which typically cost only a few euros per kg. This disparity stems largely from the low TRL and material flows estimates derived from laboratory-scale experiments. It is evident that pilot-scale testing is essential to validate (or revise) these flows and related production technology coefficients. Under the scenario studied, the new product does not demonstrate market competitiveness. Nevertheless, these findings provide a foundation for identifying key techno-economic factors driving cost components and the MPSP. Table 4 presents the results of the OLS regression, capturing the complex interplay among factors affecting the selling price. The log-log model simplifies interpretation by directly showing elasticities, illustrating how proportional changes in input variables impact costs. The results show that industry performance metrics—such as the share of raw materials in variable costs and the ratio of variable to total costs—exert significant negative effects on MPSP. As these variables improve, MPSP decreases, affirming that increased production efficiency in energy use, labour, and material consumption leads to economic advantages. A higher share of raw material costs relative to operating costs also contributes to lower MPSP, emphasizing the importance of resource optimization. Moreover, reducing the burden of fixed costs improves the competitiveness of bio-based alternatives relative to fossil-based benchmarks. The same principle applies to the relationship between average operating costs and average total costs: the smaller the contribution of fixed costs to total costs, the more competitive the bio-based alternative becomes compared to a fossil-based market price. Investment strategies should therefore consider plant scale, as larger facilities benefit from lower fixed costs per unit. Repurposing or upgrading existing infrastructure can also help reduce fixed costs and enhance the economic viability of bio-based production (Brandt et al., 2022). Regarding technological coefficients, benzene diboronic acid, thioglycerol, and epoxidised soybean oil exhibit the most significant adverse effects amongst the raw materials, meaning that improvements or reductions in their usage lead to the largest reductions in MPSP. As a result, the input costs of benzene diboronic acid and thioglycerol have the highest positive coefficients in the regression

model, indicating that increases in their prices significantly raise the MPSP of the bio-based vitrimers. Finally, variations in the economic parameters of the NPV calculation—such as the interest rate, discount rate, salvage factor, and payback period—also have a significant impact on the MPSP.

Table 3 Elasticities of the MPSP with respect to a +1 % model inputs increase

	Estimate	Pr(> t)		Estimate	Pr(> t)
<i>Industry performance</i>					
Share of ARC (***)	-1.00	0.00			
Share of AVC (***)	-0.44	0.00			
<i>Technological coefficients</i>					
Beneze diboronic acid (***)	-0.52	0.00	Biomass	-0.01	0.23
Thioglycerol (***)	-0.45	0.00	Water	0.00	0.43
Epoxidized soybean oil (***)	-0.04	0.00	Ethanol	0.00	0.50
			Acetic acid	0.00	0.50
<i>Input prices</i>					
Beneze diboronic acid (***)	0.53	0.00	Biomass	0.01	0.21
Thioglycerol (***)	0.44	0.00	Water	0.00	0.37
Epoxidized soybean oil (***)	0.03	0.00	Ethanol	0.00	0.92
			Acetic acid	0.00	0.31
<i>NPV economic factors</i>					
ρ (***)	0.03	0.00	α	0.00	0.74
r (***)	0.00	0.00	β	0.00	0.51
γ (**)	-0.01	0.00	g	0.01	0.18
τ (***)	-0.15	0.00			

Note: *** Statistical significance at <0.001 level; ** at <0.01 level; * at <0.05 level.

Among these, extending the expected break-even time period has the greatest impact in reducing the MPSP. However, a 1 % change in these economic factors yields a smaller effect on the MPSP compared to the most influential technological parameters. This reinforces the conclusion that the low TRL of the bio-based technology leaves substantial room for technological advancement and cost reduction. After establishing that industrial performance metrics are the primary drivers of the MPSP, further analysis was conducted to explore how cost elements and MPSP vary with respect to the ratio of average fixed (AFC) and variable costs (AVC), as shown in Figure 2b. A Leontief production function was applied, resulting in constant AVCs determined by input prices and technological coefficients. In contrast, other cost curves are convex, reflecting the increasing share of AVC in total costs. This convexity implies a diminishing marginal effect on the MPSP as AVC becomes more dominant in total costs. In the specific case analysed, the MPSP approaches its minimum when AVCs account for at least 60% of the average total costs, highlighting a cost-efficient plant scale where resource utilization and production efficiency are optimized.

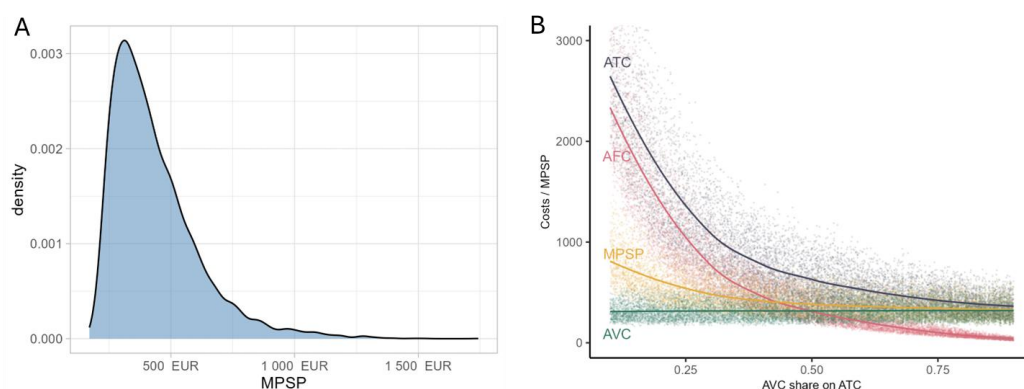


Figure 2 (A) MPSP density distribution and (B) Costs and MPSP changes for industry structures

4. Conclusions

In conclusion, this work provides an economic assessment of bio-based vitrimers production from agri-food residues using Monte Carlo simulations and a regression analysis. The scenarios modelled—based on the

process data from Cipriani et al. (2024)—offer valuable insights to inform strategic decisions in industrial and investment planning. The study confirms a cost gap between bio-based and fossil-based alternatives, stressing the need for pilot-scale testing to validate material flows and production technology coefficients derived from lab-scale experiments. Although none of the analysed scenarios demonstrate market competitiveness at this stage, the analysis offers an initial understanding of the techno-economic factors driving cost structures and pricing. Notably, industry performance metrics reveal that improving production efficiency and optimizing raw material use relative to total operating costs can enhance competitiveness. Technological coefficients and input prices—especially for benzene diboronic acid and thioglycerol—exert also a strong influence on the MPSP. Finally, the wide distribution of simulated MPSP values reflects substantial variability, highlighting significant investment risk and reinforcing the importance of technological and economic improvements for future viability. In this case, the economic performance improves when variable costs make up at least 60% of the total costs, driving the selling price towards its minimum.

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