

DEVELOPMENT OF A SIMULATION MODEL TO CARRY OUT TECHNICAL-ECONOMIC ANALYSIS OF A FOOD WASTE VALORIZATION PROCESS

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ABSTRACT

Worldwide interest in food waste has been grown over the years. According to the FAO about one third of all food produced for human consumption in the world is lost or wasted each year, amounting to about 1,6 billion tons per year. Food waste can become a source of valuable compounds which may be used as ingredients in cosmetics, pharmaceuticals, or food products. This study aims to evaluate the use of a process simulation software, specifically SuperPro Designer®, to carry out a technical-economic analysis of an orange waste valorization process. Specifically, the extraction of free sugars, essential oils, antioxidant phenolic compounds and pectin were digitally replicated by reproducing the corresponding material and energy balances. An economic and environmental assessment were carried out to evaluate the feasibility of the biorefinery modeled. The amount of orange peel processed, utilities and raw material costs were identified as significant parameters in the analyses performed. A sensitivity analysis was carried out to evaluate the profitability patterns under different operating conditions. Meanwhile, the aim of the environmental assessment is to define a disposal inventory, which is the starting point for a life cycle assessment. As a result, SuperPro Designer® can be a valuable tool in the designing and optimizing food waste treatment systems, providing detailed descriptions of the process performance, and enabling cost-effective and sustainable waste management practices. Indeed, the simulation accurately reproduced all the steps involved, identifying the total investment and the related economic parameters, as well as the outputs and the resulting disposal inventory.

1. INTRODUCTION

Food waste (FW) has become a problem of global concern that requires sustainable management strategies (Caldeira et al., 2020; Santagata et al., 2021). Valorization of FW through various processes is gaining attention to minimize waste and create valuable products (Dahiya et al., 2018). FW causes significant environmental impacts, including greenhouse gas emissions and resource depletion (J. Banerjee et al., 2017). The valorization of FW offers the potential to reduce these impacts by converting waste into valuable products, such as biofuels, bio-based chemicals, and animal feed (Bhatia et al., 2023; Imbert, 2017).

Circular economy can lead to economic benefits through the creation of new markets, job opportunities, and reduced disposal costs (Otles et al., 2015). Indeed, in Europe, the cost to dispose 1 ton of solid waste or 1 cubic meter of liquid waste ranged from 5 to more than 100€, for the period 2021-2023, including the landfill taxes (CEWEP, 2023). An effective techno-economic analysis is essential

to identify economically viable circular processes and optimize resource allocation (Ginni et al., 2021). In the context of food waste valorization, a simulation software can assess the economic feasibility, energy consumption, and environmental impact of various valorization processes (Moncada B et al., 2016). Simulation software has emerged as a powerful tool to perform techno-economic analysis of food waste valorization processes (Li et al., 2022).

Orange peels and fruit peels contain bioactive compounds that have potential applications in the pharmaceutical, cosmetic, and food industries (Maqbool et al., 2023). Indeed, simulation software can help optimize extraction processes for maximizing yield and purity of these compounds.

Anaerobic digestion is commonly employed to convert food waste into biogas (Leung et al., 2016). In this perspective, simulation software can be used to model and optimize key parameters, such as substrate composition, temperature, and hydraulic retention time to improve the efficiency of the biogas production.



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Orange peels and fruit peels can be used as feedstocks to produce bioethanol and biobutanol through fermentation processes (Sánchez et al., 2021). Moreover, for this application, the economic feasibility and process optimization of these biofuel production pathways can be evaluated using simulation software.

Simulation models heavily rely on accurate input data, which may be challenging to collect for food waste valorization processes, since they involve numerous interrelated variables. Developing accurate simulation models requires comprehensive data validation and verification against real-world operating conditions. For this reason, setting a standardized methodology for data monitoring, data collection and data reporting becomes a matter of primary importance before the implementation of the analysis on a real case study based on primary data. In this regard, the present study, based on secondary data derived from the scientific literature, may also provide a framework for future analyses on real applications.

The purpose of this study is to investigate the application of a simulation software for evaluating the feasibility of an orange peel biorefinery, providing insights into its effectiveness and potential. Specifically, the details of the valorization processes and substrate characterization were taken from the data available in the scientific literature. Thus, the process flow diagram was digitally replicated by modeling the equipment required to simulate the extraction techniques involved. As a result, economic and environmental parameters were evaluated through various scenarios by implementing a sensitivity analysis.

Section 2 describes the methodology used by first introducing the software used for the investigation, the details of the orange peel and process characterization, and the framework used to set up the economic, sensitivity and environmental analysis. For the latter, the result will be an environmental inventory to perform a life cycle assessment. Section 3 highlights the results achieved by the analyses performed and finally section 4 outlines the conclusions and future developments.

2. MATERIAL AND METHOD

2.1 Process Simulation Software

In this research SuperPro Designer® (v. 12, Intelligen, Inc., Scotch Plains, NJ, USA) was used with the aim of developing a simulation model to perform a technical-economic analysis of a suitable orange peel valorization process.

The first step in creating the simulation model was to define the physical, chemical, and environmental properties to characterize raw materials and input streams. Next, a digital flow diagram was designed by modeling all the equipment and operations involved in the process. Meanwhile, the economic and financial parameters of the biorefinery were defined as a final step. Following these stages, the software can evaluate the output streams by solving the energy and mass balances. In this way, the equipment sizing can be adjusted to define the resulting purchase cost and thus carry out the economic analysis.

The effectiveness of this simulation process lies in the fact that the economic analysis and the evaluation of the

disposal inventory were carried out by combining manufacturing, energy, and environmental operations models in the same tool.

2.2 Substrate characterization

Global orange production in the period 2022-2023 is estimated to be 5% lower at 47.5 million tons due to a lower production in the European Union (EU) and the United States (US). The EU production is forecast to decline by 13% to 5.9 million tons due to dry and warm seasons in Spain and Italy (USDA, 2023).

In 2018, 6.5 million tons of oranges were harvested in the EU. Spain was the main producer with 3.6 million tons of oranges (56% of the EU total), while the other main producers were Italy with 1.6 million tons (24% of the EU total) and Greece with 14% of the EU total (EUROSTAT, 2020).

According to (Meneguzzo et al., 2019), in 2017-2018 an amount of 36% of the global orange production was used for orange juice production, with orange waste amounting for approximately 50-60% w/w of the processed fruit. Specifically, 65% of the orange waste was characterized by peels, while the remaining 35% was internal tissues and seeds (Meneguzzo et al., 2019; Negro et al., 2017).

Table 1 shows the data collected for the modeling of the orange by-product biorefinery, with reference to Italian production in 2018.

The substrate composition, shown in Table 2, and the detailed process description were retrieved from a previous study (Tsouko et al., 2020). In particular, the available feedstock was assumed to be 7560 tons of orange peel per year, which represents about 5% of the orange peel available in Italy. According to this assumption, a quantity of 24 tons per day was evaluated, considering an operating time of 315 days per year and 24 hours per day in a continuous mode.

2.3 Model and process description

The modeled process has six distinct sections:

- Orange peel pretreatment
- Free sugars extraction
- Essential oils extraction
- Total phenolic compound extraction
- Pectin extraction
- Water and ethanol recovery and reuse

Thus, the resulting value-added compounds can be used as substrate in the cosmetic, pharmaceutical or food industries.

TABLE 1: Data collected to model the orange by-product biorefinery.

Component	Stream [tons/year]	Reference
Orange production	1 600 000	(EUROSTAT, 2020)
Orange processed in juice production	576 000	(Meneguzzo et al., 2019)
Orange waste	288 000	(Negro et al., 2017)
Orange peels	187 200	(Negro et al., 2017)
Orange peels processed by the modelled biorefinery	7560	Author's Data

Component	Percentage	Stream [kg/h]
Moisture (%wet basis)	79.1 ± 0.01	791
Solid components (%dry basis)	20.9 ± 0.01	209
Ash	3.3 ± 0.20	6.93
Protein	6.6 ± 0.30	13.86
Free sugars	50.0 ± 2.01	107.1
Essential oils	0.7 ± 0.01	1.47
Phenolics	0.6 ± 0.07	1.26
Pectin	22.0 ± 0.02	46.2
Lignin	1.2 ± 0.05	2.52
Hemicellulose	5.4 ± 0.19	11.34
Cellulose	9.2 ± 0.21	19.32

2.3.1 Orange peels pre-treatment

2.3.2 Free sugar extraction

2.3.3 Essential oils extraction

gies for the extraction of essential oils (EO) from orange by-products. Specifically, EO were mainly represented by D-Limonene. For this reason, D-Limonene properties were used to model EO properties in the software database (National Center for Biotechnology Information, 2023).

Conventional EO extraction techniques include mechanical cold pressing, water-based distillation or steam explosion, microwave steam distillation or solid-liquid extraction using conventional or organic solvents (Giwa et al., 2018; Sahraoui et al., 2011; Siddiqui et al., 2022).

In this research, the extraction of the EOs was performed by steam distillation. Specifically, 22.8 kg/min of steam (ratio 1:50 w:w) was assumed to carry out the EOs extraction for 120 minutes, obtaining 1.57 kg/h of EOs (removing up to 90% of the D-Limonene present in the peels) (Bustamante et al., 2016; Sahraoui et al., 2011).

Various methods have been reported in the literature for the extraction of phenolic compounds from orange by-products. These extraction processes are very changing to perform since phenols are very sensitive to certain conditions of high temperature and pressure (Xu et al., 2010).

Conventional solvent extraction based on ethanol was the most widely used extraction technique. There were also some interesting methods such as ultrasound assisted extraction, microwave assisted extraction, supercritical and subcritical extraction, and high hydrostatic pressure extraction, which can improve the yield of the bioactive compounds and the energy efficiency of the extraction process (M'hiri et al., 2014).

To this investigation, conventional solvent extraction was performed by using 80% ethanol. A mixture of peel powder and solvent, with a suitable ratio of 1:10 (w:v) was shaken at 200 rpm in the darkness using a mechanical stirrer for 30 minutes at 35°C (M'hiri et al., 2015). This process achieves an extraction rate of 2,19 kg/h, with 51,83% of total phenolic compounds.



2.3.5 Pectin extraction

Pectin extraction is a process that has already been consolidated at an industrial scale (May et al., 1990). In this model, the resulting stream was diluted with 2 M HCl solution with a suitable ratio of 1:20 (w:v) at 100°C for 1 hour. Subsequently, 1,5 M NaOH solution was added to adjust the pH of the resulting slurry to 4. The solid residue was separated from the mixture via decanter and the pectin-rich liquid stream was concentrated under vacuum to perform efficient concentration at low temperature to avoid pectin degradation. According to the evaluation performed, the residual solid (79,1 kg/h) were considered as a resource for other biorefineries involving hydrolysis processes of the cellulose and hemicellulose (Kulkarni et al., 2010; Tsouko et al., 2020). The extraction rate achieved is 562,20 kg/h, with 6,16% of pectin.

2.3.6 Water and ethanol recovery and reuse

A water and ethanol recovery and reuse system were simulated to reduce operating costs and to minimize the use of these valuable resources.

2.4 Economic analysis

SuperPro Designer® carries out technical-economic analysis by performing capital cost analysis, operating cost analysis, and cash flow analysis.

2.4.1 Capital cost analysis

According to (Rajendran et al., 2022), Direct Fixed Capital (DFC) should be estimated as a linear function of the equipment purchase cost (PC), considering also unlisted purchase cost. Direct cost (DC) such as piping, instrumentation, insulation, electrical facilities, buildings, yard improvement, auxiliary facilities and unlisted equipment purchase cost were expressed as a fraction of the section's total equipment PC. While side, indirect cost (IC), i.e., engineering, and construction were expressed as fraction of the section's total DC. Other cost (OC) such as contractor's fee and contingency cost were the fraction of the section's sum of DC and IC.

Capital cost analysis performed by the simulation software included other cost, such as the working cost, start-up cost and the validation cost. In this analysis, possible cost of R&D and royalties was not considered.

$$DFC = DC + IC + OC \quad (1)$$

2.4.2 Economic analysis parameters

Time evaluation and financial parameters had to be set based on the investment costs.

Specifically, the time required for the project realization and the related inflation was important to characterize the first topic.

The annual inflation rate and the net present value interest have been evaluated by considering the new European forecast. In addition, the construction and start-up period were set to 24 months, while the project lifetime was assumed to be 20 years. Construction and start-up costs were estimated to be 5% of DFC (Herrera Barragán et al., 2022).

The second issue was the financial aspect. In this case, the depreciation time was set at 10 years, the DFC outlay was defined as 30% of the DFC for the first three years, and the loan period was 10 years for the DFC and 6 years for the working capital (Kwan et al., 2018).

2.4.3 Operating cost analysis

The annual operating cost (AOC) included the cost of the raw materials, labor, consumables, quality control, quality assurance, waste treatment or waste disposal, maintenance, and utilities.

For this analysis, 10 people were assumed (including 8 operators, 1 QC analyst and 1 supervisor) to work 1720 hours per year. The total labor cost for each operator was determined by multiplying the European average labor cost, based on the European Qualifications Framework (EQF), by a lumped rate factor (it includes labor benefits or administrative costs of labor) (European Union, 2023). Furthermore, 15% of the total labor cost was allocated to cover quality control and assurance cost (Nguyen et al., 2020).

As it can be seen in Table 3, the cost of the raw material has been set individually for each material. The cost of waste disposal or waste treatment was also evaluated individually according to the material balances and the required treatment specifications.

The utilities costs were investigated by defining the contribution of each energy source. Specifically, the cost of the electricity was set at 0,51 €/kWh and the cost of producing 1 ton of steam was assumed to be 95 €/ton (Global Petrol Prices, 2023).

To cover the cost of insurance, local taxes, and factory expenses, an amount of 1%, 2%, and 5% of the DFC was assumed, respectively. Finally, the cost of maintenance has been set individually for each equipment while the depreciation cost was determined considering a depreciation period of 10 years (Herrera Barragán et al., 2022).

2.4.4 Profitability analysis

The cash flow analysis was an assessment of the annual net cash flow over the life of the project. This evaluation involved several calculations, and the results were reported in the Cash Flow Analysis Report (CFR).

Three different parameters were examined to carry out the profitability assessment. Specifically, they were:

$$\text{Gross Margin (\%)} = \frac{\text{Gross Profit } [€ \text{ years}^{-1}]}{\text{Revenues } [€ \text{ years}^{-1}]} \times 100 \quad (2)$$

$$\text{Return on Investment (ROI \%)} = \frac{\text{Net Profit } [€ \text{ years}^{-1}]}{\text{Revenues } [€ \text{ years}^{-1}]} \times 100 \quad (3)$$

$$\text{Payback time (years)} = \frac{\text{Total Investment } [€]}{\text{Net Profit } [€ \text{ years}^{-1}]} \quad (4)$$

The Gross margin is a direct measure of profit, describing the percentage of the revenues that are actual profit (2).

Return on investment is another profitability measure used to assess the feasibility of an investment or to compare the profitability of different investments (3). If an investment does not have a positive ROI, or if there are other opportunities with a higher ROI, the investment should not be undertaken.

Finally, the payback time is the inverse measure of ROI. Indeed, it is a measure of the time needed to receive the cu-

mulative net profits that exactly balances the total capital investment (4).

To perform the profitability analysis, the resulting revenues were evaluated by defining the selling price according to the references and considering the purity level achieved by the processes modeled. Assumed selling prices are reported in Table 3.

2.4.5 Sensitivity analysis

A sensitivity study has been performed to assess the predicted biorefinery performance under various operating circumstances. Based on the outcomes of the system designed using the procedure outlined in (Tsouko et al., 2020), a few significant variables were determined by considering their influence on the profitability analysis outputs. These were the demands for orange peels (kg/h) and the costs of utilities (water and steam) (€/Smc). A factorial experiment has been implemented to evaluate how these combined factors impact on the profitability outcomes. Specifically, a variation between 0 and 100 percent with a step of 25 percent has been assumed for each factor, yielding 192 potential combinations of each element. The 50 percent value of each element has been selected as the baseline. To solve the corresponding materials and energy balances, every combination has been imported into the model using the SuperPro Designer COM library. The resulting profitability metrics were compiled together into a unique data frame with the aim to provide three-dimensional graphs that illustrate the results patterns (IRR, ROI Gross Margin) with different factors.

2.5 Environmental analysis

In SuperPro Designer®, several input properties can be set to generate a disposal inventory to perform an environmental impact analysis. Specifically, the information on the disposal streams have been reported in two reports, the Environmental Impact Report (EIR) and the Emission Report (EMS).

The first defines the environmental impact of the process output streams, identifying all chemicals that are either regulated by the US Environmental Protection Agency (EPA) or marked as hazardous by the user. Each waste stream can be categorized as aqueous, organic, and solid waste or such as emissions. In addition, environmental load properties (including TOC, COD, NH₃, and others) concentrations were assessed during the analysis and an

appropriate treatment or disposal cost was assumed for each category.

To assess the effect of the chemicals, two different regulations required by US government were considered, EPCRA Section 313 and 33/50 Program. According to the first regulations, facilities were required to report annually a Toxic Chemical Release Inventory, which includes all the releases to the environment and other waste management of toxic chemicals that occurred during the previous calendar year (EPA, 2023).

Pollution indices were reported in the last section of the EIR report. These indices are representative of the environmental performance of the developed process:

$$Y1 = \frac{\text{Total Waste [kg]}}{\text{Main Revenue Stream [kg]}} \quad (5)$$

$$Y2 = \frac{\text{Total Waste [kg]}}{\text{Raw Material [kg]}} \quad (6)$$

The first index represents the ratio of the total amount of waste generated per kg of the main revenue stream processed, which is in this case the pectin rich liquid due to the large volume. The second index considers the same amount of waste generated but related to kg of raw material used. The analysis carried out provides also specific index to assess the ratio between the single stream waste (i.e, solid, aqueous, and pollutant) generated and the kg of main revenue stream or raw material.

The second report generated (EMS) provides information on the air pollutant impacts related to the whole process or individual procedure. For each air pollutant identified, the procedure/operation averaged component rates, the time-averaged component rates, and the total amounts have been assumed.

As a result, the outputs of this analysis can be used to perform a life cycle assessment with the aim of assessing the sustainability of the processes involved.

3. RESULTS AND DISCUSSION

3.1 Capital Costs Analysis Result

The results of capital cost analysis carried out by using the equation (1) are reported below. As can be seen, the amount of the DFC is more marginal than the annual operating cost.

- DFC = 7 129 000 €
- AOC = 38 855 000 €

TABLE 3: Raw material cost and revenue for each by – product expressed as €/kg.

Raw Material	Purchase Cost [€/kg]	Reference	Revenue	Selling price assumed [€/kg]	Reference
Orange peels	0,0025	(S. Banerjee et al., 2022)	Free sugars	1	(Foodcom, 2023)
HCl (37%)	0,3	(MERCK, 2023)	Essential oils	10	(Cbi, 2023)
NaOH	0.3	(MERCK, 2023)	Total phenolic compound	20	(Fisher scientific, 2023)
Ethanol	0.62	(Trading Economics, 2023)	Pectin rich liquid	10	(MERCK, 2023)
Water	1.5E-3	(ARERA, 2023)	Solid residual to Hydrolise	3	(MERCK, 2023)

3.2 Operating Costs Analysis Result

The value of the annual operating cost (AOC) based on the analysis carried out by the simulation software is 38 855 000 €. Figure 2 shows the distribution of the different item cost related to the AOC to identify the main cost item, which is the cost of utilities (78%), followed by the cost of the raw materials (17%), the labor-dependent cost (2%), the cost of the depreciation (2%), and the other facility – dependent cost (2%).

3.3 Profitability Costs Analysis Result

The modeled process gave a high ROI and a very short payback time. These highlight the profitability of the process which recovers over 60% of the initial investment in 1.57 years with a gross margin of 17.91%. As reported below:

- Gross margin (%) = 17,91%
- ROI (%) = 63,69%
- Payback time (years) = 1.57 years

3.4 Sensitivity Analysis Result

The annual operating cost section highlights how the utilities and raw materials are the major operating cost items. Indeed, the high influence of the former is due to the large amount of steam and water required to perform the heat transfers throughout the process. Similarly, the costs of the raw materials are also significant due to the large amount of water required to process the orange peels. According to the capital cost section, the DFC is linearly dependent on the equipment purchase cost, which is influenced by the volume of orange peel processed by the biorefinery.

As a result, the orange peels demand, the steam production costs, and the water supply and distribution costs were assumed as significant factors to carry out the sensitivity analysis. Figures 2 (a-b-c) show the patterns of gross margin, ROI, and payback time related to the combination between the identified factors.

3.5 Environmental Analysis Result

The performed environmental analysis highlights different indices, reported below, which show how much waste has been generated in relation to the main product of the biorefinery and the raw materials processed. The results show that 1.33 kg of waste was generated to produce 1 kg of pectin rich liquid. At the same time, according to the equation 6, total waste represents the 50% of the processed raw material. As it can be seen below, the main waste stream is represented by the aqueous stream.

$$Y1 = 1.33 \frac{\text{kg of waste}}{\text{kg of main revenue stream}}$$

$$Y2 = 0.50 \frac{\text{kg of}}{\text{kg of raw material}}$$

4. CONCLUSIONS

Waste management and waste valorization are the key drivers for reducing the environmental impact and increasing the economic growth. Indeed, several value-added products can be produced by valorizing the FW such as

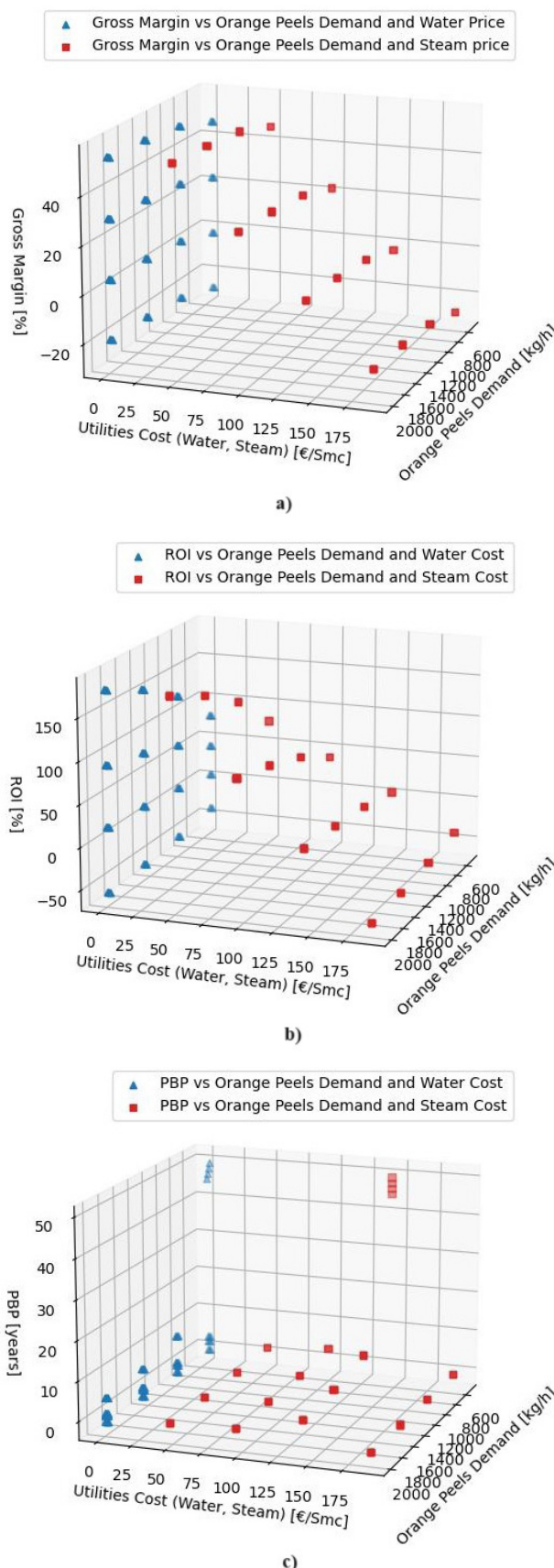


FIGURE 2: a) Gross margin vs. orange peel demand, water, and steam costs; b) ROI vs. orange peel demand, water, and steam cost; c) Payback time vs. orange peel demand, water, and steam costs.

biofuels, bio – based chemicals, and animal feed. Specifically, the attention on the bioactive compounds contained in fruits and agri-food products has grown over the years since they have potential applications as ingredients in the pharmaceutical, cosmetic and food industries. The scientific literature shows how several strategies for the extraction of these substances from FW have been investigated on a laboratory scale. With the aim of scaling up these processes to a pilot plant or industrial level, a technical-economic analysis had to be carried out to assess their feasibility. At the same time, the evaluation of some environmental parameters related to the processes involved is an essential step for the optimal design of a valorization process. The mentioned evaluations can be performed by using the simulation software to produce a digital replica capable of reliably reproducing the characteristics of the real processes.

The aim of this study is to investigate the application of a simulation software, SuperPro Designer®, to assess the feasibility of an orange peels valorization biorefinery, providing insight into its effectiveness and potential. Specifically, scientific evidence highlights how the substrate investigated can be a source of free sugars, essential oils, antioxidant phenolic compounds, pectin, cellulose, and hemicellulose. The modeled biorefinery was able to produce all the mentioned compounds by involving a series of extraction strategies.

As the first step, all the raw material and stream properties (physical, chemical, economic, and environmental properties) were initialized. In addition, all the economic, financial, and environmental parameters were defined with the aim of performing the technical-economic analysis and generating the disposal inventory. Next, all the equipment involved in the process was modeled to replicate the corresponding process flow diagram. At this point the software can evaluate the output streams by solving the energy and mass balances. As a result, the sizing of the equipment can be adjusted to define the resulting purchase cost and thus perform the economic evaluation. The latter was based on the direct fixed capital cost and annual operating cost. In particular, the former was characterized by the direct and indirect costs, which were a linear function of the equipment's purchase cost. Meanwhile, the most influential annual operating costs were raw materials and utilities costs. Three different parameters, gross margin, return on investment, and payback time, were examined to evaluate the profitability performance. Furthermore, a sensitivity analysis was performed to evaluate the patterns of the profitability indices by varying the parameters that have a relevant influence on the economic evaluation.

The simulation software provided the environmental impact and emission reports. From these, two different indices were identified to preliminarily quantify the waste generated. Specifically, the first described the ratio between the amount of waste and the stream with the highest mass flow, while the second showed the ratio between the amount of waste and the raw material processed. In addition, the resulting reports provided an environmental inventory useful for further analysis focused on a life cycle assessment.

Digging deeper into the results, valorization processes

represent a sustainable strategy to address the pressing issue of the FW. In this perspective, simulation software has emerged as a valuable tool for technical-economic analysis of food waste valorization processes. Potential assessments include economic viability, resource optimization, and environmental inventory management.

Despite some limitations, ongoing advances in simulation software and data availability hold promising prospects for further improving the effectiveness and accuracy of such analysis. Future research should focus on refining simulation models and integrating advanced technologies to support sustainable food waste valorization practices. Data collection and reporting on waste recovery processes also needs to be improved and standardized.

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