Exploring Biorefinery designs for Agricultural Waste with Stochastic Optimization

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Abstract

As the push for designing sustainable processing plants increases, the need for adequate tools to analyze and optimize these plants becomes paramount. Particularly the agricultural sector is in need of new and innovative biorefineries capable of handling the generated waste and transforming them in to added value products. Superstructure optimization offers an elegant solution to explore many alternative processing routes with one or multiple objectives in mind such as, sustainable and financial criteria. Various user friendly and accessible superstructure optimization tools for process design already exist but do not provide the capability to make decisions under uncertainty. This contribution aims to extend the OUTDOOR software package to handle superstructure optimization problems under uncertainty, using a 2-stage approach with fixed recourse. A case study is presented showcasing the extended OUTDOOR application on a processing plant that transforms potato peels into added value products. From the stochastic solution the most beneficial processing route, while considering all the uncertainties, lies in the production of phenolic compounds next to the production of starch, generating an expected revenue of 0.89 million euros per year. The value of perfect information (EVPI) was calculated to be 0.02 million euros, indicating the price of perfect information. The value of the stochastic solution (VSS) was 0 euros, indicating that the produced flowsheet is the most optimal one, across all uncertain scenarios.

**Keywords**: 2-Stage stochastic problem with fixed recourse, Superstructure optimization, OUTDOOR, optimization under uncertainty

* 1. Introduction

In the current global scenario, where sustainability is of paramount concern, the agricultural sector is critically situated at the nexus of ensuring food security, preserving environmental integrity, and executing waste management. One of the pressing issues is the management of agricultural waste, with a specific focus on diminishing its environmental impact through reduced methane emissions, while advancing a circular economy paradigm (Gontard et al., 2018).

Biorefineries are pivotal in this context, tasked with the valorization of agricultural waste through the extraction of valuable compounds. However, the development of processing routes to utilize agricultural waste remains a complex challenge. This complexity stems from the rapid emergence of new technologies and the significant unpredictability associated with the efficiencies of processes and the variability of feedstock attributes.

Superstructures are mathematical frameworks that encapsulate all potential design pathways and configurations for a given system. Optimization of these superstructures facilitates the identification of the most effective configuration (e.g., in terms of costs, environment or performance) within the bounds of predefined constraints and objectives (Mencarelli et al., 2020). Several user-friendly computational tools, including SUPER-O, O2V, and OUTDOOR, harness the power of superstructure optimization to systematically evaluate process design alternatives (Bertran et al., 2017; Gargalo et al., 2022; Kenkel et al., 2021). However, these tools lack a crucial feature: they do not effectively address uncertainty. Given the variable nature of feedstock properties, process parameters, and market prices, designing bioprocessing plants that can withstand these uncertainties is essential, making optimization under uncertainty a crucial aspect. To address this gap, the OUTDOOR software tool has been extended to incorporate uncertainty into the optimization of superstructures as a 2-stage stochastic linear program with recourse. This enhancement streamlines decision-making for the design of process flowsheets by allowing robust process development under uncertainty, providing a more resilient and user-friendly approach to biorefinery design. The upgraded OUTDOOR tool thus stands to significantly impact the sector by enabling the development of biorefinery configurations that are better equipped to handle the uncertainties inherent in waste management of the agricultural sector.

* 1. Methods and Materials
		1. Superstructure design

The configuration of the superstructure in this study largely adheres to the framework established by Kenkel et al. (2021). The software package, developed in Python, employs an Excel wrapper for data aggregation and processing to establish a superstructure model.

This model encompasses detailed mass and energy balances, operational (OPEX) and capital expenditures (CAPEX) and provides preliminary estimates of CO2 emissions and freshwater consumption for each unit operation under consideration. For an in-depth understanding of the mathematical model underpinning OUTDOOR, readers are directed to the detailed exposition in Kenkel et al. (2021).

* + 1. 2-Stage stochastic problem with fixed recourse

In this study, a two-stage stochastic program with recourse is proposed to address uncertainties inherent in the superstructure model (Birge and Louveaux, 2011). The uncertain parameters include reactor efficiencies, separation efficiencies, product and substrate prices, reactor yields, and feedstock composition. In a two-stage stochastic program, there are two types of decision variables: In the first stage, decisions regarding the choice of unit operations are made. In other words, a decision of the plant layout needs to be made before the uncertainty manifests, i.e., “here and now”. These decisions are irreversible and must be taken without complete knowledge of the future. The second stage involves variables that become apparent post the occurrence of uncertain events or when recourse actions are required to maximize the objective function. In our model, these actions include the diversion of streams to different unit operations, aligning with the “wait and see” principle of optimization. The two-stage stochastic optimization problem can be represented in mathematical notation as follows:

|  |  |
| --- | --- |
| $$min Z=f(x,y)+\sum\_{k}^{}E\_{k}[q(x,y, ξ\_{k},)]$$ | (1) |
| $$s.t. g\_{k}\left(ξ\_{k},x,y\right)\geq 0$$ | (2) |
| $$h\_{k}\left(ξ\_{k},x,y\right)=0$$ | (3) |
| $$x^{L}\leq x\leq x^{U}$$ | (4) |
| $$x\in R   y \in \left\{0,1\right\}$$ | (5) |

where the objective function *Z* is a dependent on decision variables *x,* *y*, and the probability *Ek* of scenario *k* occurring. The uncertain parameters per scenario are denoted as *ξk*. In our model, equal probability of each scenario *k* occurring, is assumed. The inequality constraints *gk(ξk, x, y)* represent operational boundaries, while the equality constraints *hk(ξk, x, y)* encompass mass and energy balances and logical constraints. The function *f(x, y)* reflects the costs associated with the first-stage decisions. Conversely,
*q(x, y, ξk)* signifies the expected costs of each subsequent action or second-stage decision, in response to the realized uncertainties. The model also includes boundary constraints, ensuring that continuous decision variables remain within realistic limits, such as prohibiting negative flows (Eq. 4).

In the context of our study, *Z* signifies the Earnings Before Interest and Taxes (EBIT), calculated as the revenue from sales minus the capital (CAPEX) and operating expenses (OPEX). CAPEX, associated with f*(x, y)*, primarily depends on the first-stage integer decision variables y, which indicate the selection of specific technologies and is calculated with linearized economies of scale. The revenue and OPEX, represented by *q(x, y, ξk)*, are influenced by the uncertain scenario parameters *ξk* and the continuous variables *x*, which denote, for example, mass flows and energy consumption. The EBIT is then derived as the expected value from the weighted sum of the revenue and OPEX subtracted by the CAPEX.

In the extended version of the OUTDOOR software, the integration of uncertainties into the optimization framework is efficiently facilitated by the Excel wrapper. Due to the exponential increase in model size with each added uncertain parameter, strategic grouping of certain parameters can be employed to mitigate this growth. For instance, if starch and lipid contents in potato peels exhibit an inverse relationship—high starch content correlating with low lipid percentage—this correlation is consistently reflected across all scenarios. In effect, scenarios featuring above-average lipid and sugar content in potato peels are excluded. This approach not only maintains the model at a feasible scale but also substantially reduces computational time.

* + - 1. VSS and EVPI: Key Metrics in Stochastic Decision-Making

Prior to the optimization, every possible scenario undergoes a feasibility check via deterministic optimization. Scenarios deemed infeasible are excluded, streamlining the stochastic optimization process. This step also helps in determining the feasibility bounds for the process parameters that exhibit uncertainty. Furthermore, the Expected Value of Perfect information (EVPI) can be calculated from these deterministic solutions. EVPI is a measure in stochastic optimization that quantifies the maximum amount a decision-maker would be willing to pay for having perfect information about uncertain parameters, before making a decision. It represents the difference in the expected outcome between the ideal scenario where uncertainty is resolved before the decision and the realistic scenario where decisions are made under uncertainty (Birge and Louveaux, 2011). The EVPI is calculated as followed:

|  |  |
| --- | --- |
| $$EVPI=EVwPI -EVSS$$ | (6) |

where EVwPI (Expected Value with Perfect Information) is the average of all the solution of the deterministic optimization problems as if the realizations were known in advance. The EVSS is the Expected Value of the Stochastic Solution.

A second metric that can be calculated is the Value of the Stochastic Solution (VSS). The VSS quantifies the benefit of using a stochastic model over a deterministic model (which uses fixed, often average values of uncertain parameters). In other words, the VSS reflects the improvement in expected performance (e.g., cost reduction, increased efficiency) achieved by accounting for uncertainty in the decision-making process (Birge and Louveaux, 2011). The VSS is calculated as followed:

|  |  |
| --- | --- |
| $$VSS=EVDS - EVSS $$ | (7) |

where EVDS is the Expected Value of the Deterministic Solution which is the solution from the deterministic equivalent of the problem by replacing the uncertain parameters with their average values.

* + 1. Case study description

To demonstrate the capabilities of the updated OUTDOOR framework under uncertainty, a superstructure case study was developed, focusing on the valorization of potato peels (Figure 1). The superstructure begins with the extraction of starch, a relatively straightforward and valuable product derived from potato peels. This process involves grinding the peels into a pulp and then separating the liquid fraction, from which starch is obtained. The remaining pulp fraction, still rich in valuable components, is then considered for further processing into three potential products through different routes: i) Phenolic compounds, targeted as antioxidants for the food industry, ii) bioethanol at 85% volume concentration and iii) polylactic acid (PLA), a type of biopolymer. Moreover, the feasibility of producing methane via anaerobic digestion is also explored. This methane could potentially be utilized to generate electricity and/or heat, necessary for operating the other unit processes. The goal of the optimization problem is to assess which product streams and combination of technologies maximize the total yearly profit defined as the EBIT. Further assumptions made is that the plant is capable of processing 1 ton of potato peels per hour and is operational 8000 hours per year. The complete superstructure with all unit processes can be seen in Figure 1. In this superstructure 4 grouped sources of uncertainty are considered: i) the composition of the potato peels, ii) the conversion efficiency of carbohydrates to ethanol in the fermentation unit, iii) the seperation efficiency of phenolic compounds in the extraction units and iv) the market prices of products.



Figure 1: Superstructure of the biorefinery. Green boxes are input streams, yellow boxes are the product outputs, blue boxes represent unit processes and blue circles are where streams can be split.

OUTDOOR automatically creates unique scenarios, where each combination of uncertain parameters is possible. For each parameter in a scenario, three potential values can be represented: the expected value or the expected value adjusted by a predefined standard deviation (either plus or minus). This approach resulted in the creation of 243 distinct scenarios. The stochastic model is then solved where all the unique scenarios are represented. The problem presents itself as a Mixed Integer Linear Problem (MILP) with 131.012 variables, 2220 integer variables and 238.633 constraints and is solved using the Gurobi solver (Gurobi Optimization, 2023) in Python (version 3.10).

* 1. Results and Discussion
		1. Stochastic outcome of the case study

The two-stage stochastic optimization problem was integrated into the OUTDOOR framework, as outlined in the methodology section. The case study was executed on a 12th Gen Intel(R) Core(TM) i7-1255U processor, with the solution obtained in 857 seconds. The optimized design of the superstructure, displayed in Figure 2, showcases the minimum, mean, and maximum flow rates through each unit process. The expected EBIT stands at 0.89 million euros per year. Notably, the range of EBIT spans from a minimum of 0.22 million euros to a maximum of 2.57 million euros, underscoring the impact of uncertainties on economic outcomes. A consistent outcome across all scenarios is the co-production of phenolic compounds alongside starch, despite the relatively low production rate of phenolic compounds, averaging at 1.17 kg/h. This decision is largely influenced by the high market value of these compounds. As depicted in Figure 2, the production rate of phenolic compounds is markedly sensitive to the scenario being considered (indicated by the deep red colored line). This sensitivity is attributed to the variability in the efficiency of the extraction process and the fluctuating composition of phenolics, highlighting the significance of incorporating uncertainties in process optimization. Another curious observation is that the generation of electricity or heat, through the combustion of methane, is not considered, suggesting that the savings on energy do not justify the capital investment required to install these unit processes.

* + - 1. Evaluating the stochastic solution

To assess the robustness of the stochastic solution, two key metrics were computed: the Expected Value of Perfect Information (EVPI) and the Value of the Stochastic Solution (VSS). The EVPI was calculated at 0.02 million euros, with the EVwPi being 0.87 million euros. The EVPI indicates the potential benefit of obtaining perfect information about uncertainties before making decisions. In practical terms, this suggests that investing up to this amount in research to improve process reliability or in economic tools for more accurate market price predictions would be justifiable. Conversely, the VSS came out to be 0 euros, implying that under every considered scenario, constructing the refinery as per the stochastic solution is the optimal strategy. This result can primarily be attributed to the fact that, regardless of the efficiency and yield variations in phenolic compound production, the high selling price of these compounds invariably makes their production the most lucrative option.

* + 1. Future work

The next step in extending OUTDOOR's capabilities is to include multi-criterion decision-making tools under uncertainty. Such extensions will allow for a more comprehensive understanding and effective balancing of various objectives such as cost, environmental impact, and process reliability, even in the face of uncertainties.



Figure 2: The flowsheet generated by the solution of the stochastic optimization problem. Green boxes are inputs, yellow boxes are outputs, blue boxes are unit operations. The darker red lines represent streams which are more susceptible to uncertainty.

* 1. Conclusions

OUTDOOR has been successfully updated for superstructure optimization under uncertainty, using a two-stage stochastic optimization with fixed recourse. This solution yields a process flowsheet and adapts stream division according to unfolding uncertain scenarios, alongside metrics for solution assessment. Applied to a case study for valorizing potato peels, OUTDOOR pinpointed an optimal and robust biorefinery design for phenolic compounds and starch production, with an expected EBTI of 0.89 million euros per year. The calculated EVPI is 0.02 million euros, indicating the value of perfect information, while a VSS of 0 euros suggests the flowsheet's optimality under all conditions. With this updated version of OUTDOOR a user-friendly approach integrating uncertainty into process design, is achieved, facilitating the development of biorefinery configurations capable of handling uncertainties.

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