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Simulation, technical-economic evaluation and risk analysis of the purification of different bio-oils obtained by the fast pyrolysis process

Simulação, avaliação técnico-econômica e análise de riscos da purificação de diferentes bio-óleos obtidos pelo processo de pirólise rápida

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Abstract
Biomass is a natural compound that originates from various forms of organic matter. One way to transform biomass into value-added products is through the fast pyrolysis process, which is a thermochemical process that produces solid, liquid and gaseous compounds. The main product of this process is the bio-oil, found in the liquid phase and containing a wide range of value-added compounds that can be obtained through extraction and distillation. Simulation is an important tool for predicting, modeling and understanding the feasibility of the desired process, along with economic analysis of risks and uncertainties, which are useful techniques for studying the feasibility of projects. In this context, this work aimed to carry out the simulation using the Aspen Plus ® process simulator, the analysis of economic viability and the analysis of risks and uncertainties of the process of separation and purification of bio-oil compounds, derivatives of wood from eucalyptus, eucalyptus residues and sugarcane bagasse. After completing these steps, the project achieved a good result, with desired products being obtained with a considerable degree of purity for commercialization. Economically, all processes were viable, obtaining a good return on investment and a short payback period, despite the high costs involved. Even considering risks and uncertainties, including the variation in the cost of raw materials and production capacity, the investment still returned good results, demonstrating that the project is economically viable even under these circumstances.
Keywords: Aspen Plus. Biomass. Bio-oil. Separation.

Resumo
A biomassa é um composto natural que se origina de diversas formas de matéria orgânica. Uma forma de transformar biomassa em produtos de valor agregado é através do processo de pirólise rápida, que é um processo termoquímico que produz compostos sólidos, líquidos e gasosos. O principal produto desse processo é o bio-óleo, encontrado na fase líquida e contendo uma ampla gama de compostos de valor agregado que podem ser obtidos por extração e destilação. A simulação

é uma importante ferramenta para prever, modelar e compreender a viabilidade do processo desejado, juntamente com a análise econômica de riscos e incertezas, que são técnicas úteis para estudar a viabilidade de projetos. Neste contexto, este trabalho teve como objetivo realizar a simulação utilizando o simulador de processos Aspen Plus®, a análise de viabilidade econômica e a análise de riscos e incertezas do processo de separação e purificação de compostos de bio-óleo, derivados de madeira de eucalipto, resíduos de eucalipto e bagaço de cana. Após a conclusão dessas etapas, o projeto obteve um bom resultado, sendo obtidos os produtos desejados com considerável grau de pureza para comercialização. Economicamente, todos os processos foram viáveis, obtendo um bom retorno do investimento e um curto período de retorno, apesar dos elevados custos envolvidos. Mesmo considerando riscos e incertezas, incluindo a variação no custo das matérias-primas e na capacidade de produção, o investimento ainda retornou bons resultados, demonstrando que o projeto é economicamente viável mesmo nestas circunstâncias.
Palavras-chave: Aspen Plus. Biomassa. Bio-óleo. Separação.

1. Introduction

With the growth of the population and its technological aspirations, energy demand is increasing rapidly. In the early twentieth century, world energy production focused on the coal and oil industries, but with the rampant exploitation of natural reserves and the issue of greenhouse gas emissions, interest in sustainable energy production arose. Renewable energy sources, such as biomass, play a key role in the energy, environmental and socio-economic landscape (Demirbas, 2005; Evaristo *et al*., 2022).

Biomass pyrolysis is a process that has been studied. It promotes thermal decomposition of biomass in the absence of oxygen to produce solids, liquids and gaseous products. The design of the pyrolysis reactor, the operating parameters (temperature, heating speed, residence time, pressure and catalyst), the type of biomass and its physical characteristics (particle size, shape and structure), can affect the yield and properties of the product formed (R. Kumar *et al*., 2020) and, consequently, the efficiency of the process.

The liquid product obtained from pyrolysis (bio-oil or pyrolytic oil) has a dark brown color and characteristic odor, in addition to being considered a complex mixture of water and organic compounds (Stedile *et al*., 2015). In its composition, several compounds have already been identified, such as acids, alcohols, aldehydes, esters, ketones, phenols, furans, hydrocarbons and nitrogenates (Guo *et al*., 2015; Lazzari *et al*., 2016), which gives it great potential for application as a source of raw material for chemicals, as well as in the fuel industry. The purification of bio-oil is an attractive route to obtain the compounds present in it, since they have added values and great potential for use in numerous areas, such as chemistry, biochemistry, health, agronomy and even gastronomy (Campos-Franzani *et al*., 2020; Drugkar *et al*., 2022; Hassen-Trabelsi *et al*., 2014; Wang *et al*., 2010).

The chemical industry uses modeling and simulation as tools that offer the possibility of predicting operating conditions or simulating equipment, without interfering with the process. In addition to saving inputs, simulating a production process before implementing it on a large scale also saves time (Deng *et al*., 2019; Liu *et al*., 2022; Rosha *et al*., 2022; Yamini *et al*., 2022).

The present work aimed to simulate the process of separation of bio-oil compounds derived from fast pyrolysis of different biomasses, using the Aspen Plus® process simulator, in addition to evaluating the technical-economic and risk feasibility of the process.

2. Material and methods

2.1. Simulation

To simulate the separation of the liquid fraction from the fast pyrolysis product, the commercial simulator ASPEN PLUS version 12.1 was used. Through the literature, the compositions of three different bio-oils were obtained: derived from eucalyptus wood (G. Kumar *et al*., 2010), eucalyptus residue (Klafke, 2018) and sugarcane bagasse (David *et al*., 2018), all

obtained by the fast pyrolysis process. Due to the different compositions of the bio-oils, three different scenarios 1, 2 and 3 were simulated, respectively.

In the Properties environment, the components used in the simulations were inserted. The choice of the thermodynamic package was determined from adjustments during the simulations. The steps involved in the separation process were: extraction using hexane as solvent and distillation, both for solvent recovery and for obtaining compounds. In some simulations it was necessary to use a distillation column prior to extraction to separate components more volatile than the solvent.

To prepare the process simulations, literature works (Chan *et al*., 2020; Jiang *et al*., 2021; Shahbaz *et al*., 2022) were used as reference to define the operational parameters, such as temperature and pressure, and the bio-oil compositions available in these works.

The addition of each equipment in the simulations was made directly in the process flowchart, and the material currents between each of the equipment were inserted so that all equipment was connected, thus representing the entire bio-oil purification process. The configured currents were only the input currents in the process, and the others are the result of the unit operations involved.

The bio-oil feed rate in each of the simulations was 100 kg/h, with their respective compositions and fractions. In the process there was also a solvent feed stream, which joined the recycle stream, resulting in a solvent feed rate of 100 kg/h.

After assembling the process flowchart and defining the input currents and the operational conditions of the process, the simulations were carried out and the output currents were obtained.

2.2. Economic analysis

The economic evaluation consisted of the estimation of the investment necessary for the construction of the bio-oil purification process plant derived from different biomasses, with the objective of obtaining compounds of aggregate values, and the estimates of revenue in the face of a given economic scenario. The simulations were carried out with a capacity of 100kg/h of bio-oil, operating at 7,920 h/year, corresponding to 330 annual days.

The economic analysis was carried out taking into account the cost of capital for the construction of the industrial plant, profitability analysis of the proposed process, analysis and selection of the best process for generating the final product, sale value and analysis of the economic potential of the product in the market. With the help of the Aspen Plus process simulator, the costs of the process equipment and utilities were estimated. From these data, the economic analysis was carried out with the aid of spreadsheets (Plant Design and Economics for Chemical Engineers, 2003; Turton *et al*., 2009).

2.3. Risk and uncertainty analysis

The values used in the economic evaluation are subject to uncertainties. Thus, considering the existence of uncertainties in variables such as investment, raw material costs, industrial production, among others, means admitting the presence of risk in decision-making about the relevance of the project. The result of the risk analysis includes a series of information about the potential risk associated with the decision or investment (Watanabe & Bonomi, 2021). A widely used technique for risk and uncertainty analysis is Monte Carlo Simulation. It consists of using random numbers as inputs to interactively evaluate a deterministic model. This method is especially useful when the model is complex, non-linear or when it presents several uncertainty parameters (Lima *et al*., 2008). As a result, probability distribution plots of the simulated results are obtained, including the mean, standard deviation, and number of results.

In this work, Monte Carlo Simulation was used to evaluate the uncertainties in the economic feasibility analysis of the process for each type of bio-oil considered. For this, spreadsheets already adapted were used to generate random values for probability distribution of the Net Present Value (NPV) of the Project as a function of the cost of raw material (bio-oil). For the risk analysis carried out due to the variation in the cost of raw materials, a variation of +20% of the cost value of bio-oil was considered.

3. Results and discussion

3.1. Simulation results

The NRTL model is based on experimental data, however, because the Aspen database does not present experimental data among the mixture of bio-oil compounds, and these data are also not available in the literature, the extraction column simulation was not successfully completed, presenting results without the presence of errors. To try to solve the problem, and possibly obtain a satisfactory result, a separator was used to simulate the extraction column and obtain only the desired component, using a solvent that would not have affinity for this compound.

3.1.1. Simulation 1

Later inserting the blocks, chains and their respective configurations, it was possible to obtain the Process Flow Diagram (PFD) of Simulation 1 presented in Figure 1, referring to the refining of eucalyptus wood bio-oil.

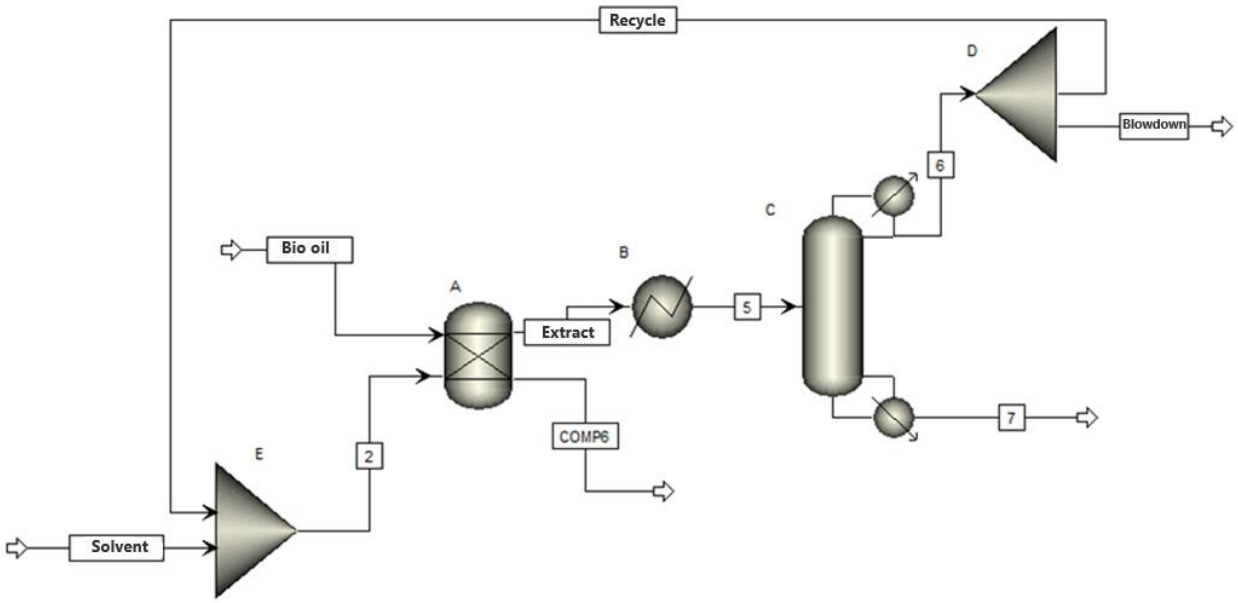

Figure 1 - Simulation 1 Process Flow Diagram (Authors, 2024).

Table 1 – Description of the blocks used in Simulation 1 (Authors, 2024).

Name in the simulator	Block ID	Description
SEP	A	Simulates an extraction column to separate the COMP6 component from the others, due to solvent incompatibility.
HEATER	B	Simulates a heat exchanger to raise the temperature prior to entry into the distillation column.
RADFRAC	C	Simulates a distillation column to separate the solvent from the other products.
FSPLIT	D	Simulates a separation equipment to separate a fraction of the stream and recover it to the process.
MIXER	E	Simulates a mixer to integrate the recycle stream into the input solvent.

The component of choice for refining was COMP6 (3-Hydroxy-4-Methoxybenzoic Acid), from which, when obtaining the product stream, the next step was to recycle the solvent through a distillation column. The undesired components were routed to stream 7. Table 2 shows the results obtained in Simulation 1.

Table 2 – Composition of Simulation 1 currents (Authors, 2024).

No. of compounds	Aspen Nomenclature	Compound	Bio oil	Solvent	Recycle	Blowdown	Comp6
			Mass flow (kg/h)				
			100.00	1.00	99.00	1.00	14.93
			Fraction				
1	FURFU-01	2-Furan Carboxaldehyde	4.54	-	-	-	-
2	GUAIA-01	2-Methoxyphenol	9.28	-	-	-	-
3	4-MET-01	1-Hydroxy-2-Methoxy-4-Methyl Benzene	11.05	-	-	-	-
4	4-ETH-01	4-Ethyl-2-Methoxyphenol	12.42	-	-	-	-
5	SYRIN-01	2,6-Dimethoxyphenol	13.55	-	-	-	-
6	COMP6	3-Hydroxy-4-methoxybenzoic acid	14.93	-	-	-	1.00
7	COMP7	3-Furan Carboxylic Acid	16.00	-	-	-	-
8	COMP8	2,6-Dimethoxy 4(2-Propynyl)Phenol	18.23	-	-	-	-
9	N-HEX-01	n-Hexane	-	1.00	99.00	1.00	-

We can observe through the results of the simulation that the product desire (COMP6) was successfully obtained, and 99% of the solvent used in the process can be recovered.

3.1.2. Simulation 2

Right away inserting the blocks, chains and their respective configurations, it was possible to obtain the Process Flow Diagram (PFD) of Simulation 2 presented in Figure 2, referring to the refining of bio-oil from eucalyptus waste.

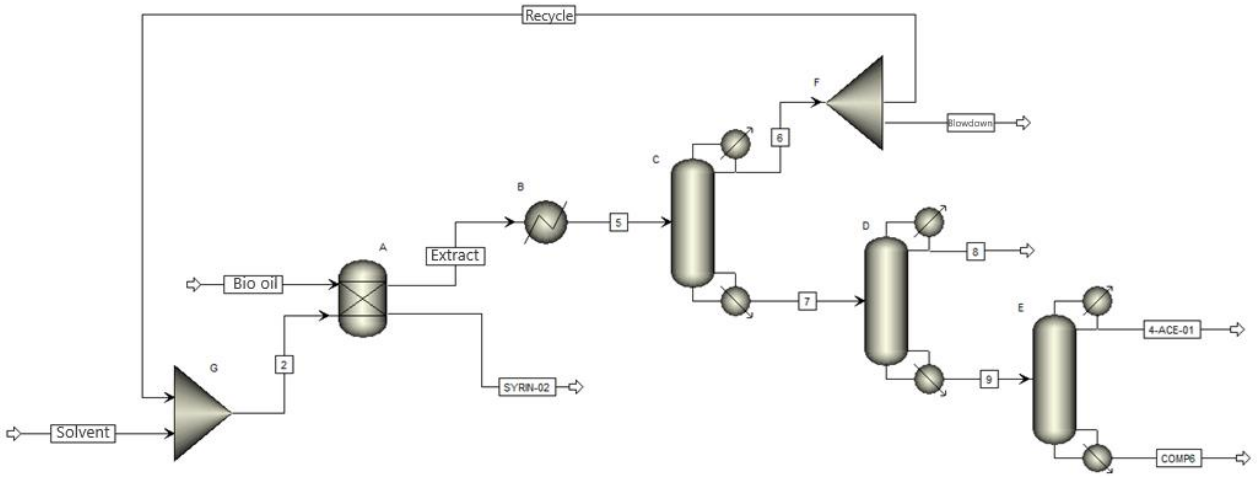

Figure 2 - Simulation 2 Process Flow Diagram (own authorship)

Table 3 describes the unit operations considered in Simulation 2.

Table 3 – Description of the blocks used in Simulation 2 (Authors, 2024).

Name in the simulator	Block ID	Description
SEP	A	Simulates an extraction column to separate the COMP6 component from the others, due to solvent incompatibility.
HEATER	B	Simulates a heat exchanger to raise the temperature prior to entry into the distillation column.
RADFRAC	C	Simulates a distillation column to separate the solvent from the other products.
RADFRAC	D	Simulate a distillation column to separate a fraction of compounds.
DISTL	E	Simulates a distillation column to separate the 4-ACE-01 component from the other compounds.
FSPLIT	F	Simulates a separation equipment to separate a fraction of the stream and recover it to the process.
MIXER	G	Simulates a mixer to integrate the recycle stream into the input solvent.

Table 4 shows the results of the currents later the simulation has been performed.

Table 4 – Result of Simulation 2 currents (Authors, 2024).

No. of compounds	Aspen Nomenclature	Compound	Bio oil	Solvent	Reciclo	Blowdown	Syrin-02	4-ace-01
			Mass flow (kg/h)					
			100.00	10.00	90,00	10.00	6.08	12.22
			Fraction					
1	1-MET-01	1-Methylimidazole	0.53	-	-	-	-	-
2	2(5H)-01	2(5H)-Furanone	0.63	-	-	-	-	-
3	COMP3	2-Hydroxy-2-cyclopenten-1-one	3.81	-	-	-	-	-
4	3-MET-01	3-Methyl-2-Cyclopenten-1-one	0.43	-	-	-	-	-
5	PHENO-01	Phenol	0.53	-	-	-	-	-
6	COMP6	3-Methyl-2,4-Imidazolidinedione	2.17	-	-	-	-	-
7	COMP7	2-Hydroxy-3-Methyl-2-Cyclopenten-1-one	2.28	-	-	-	-	-
8	O-CRE-01	2-Methylphenol(o-Cresol)	0.46	-	-	-	-	-
9	2(3H)-01	γ-Caprolactone	0.56	-	-	-	-	-
10	P-CRE-01	4-Methylphenol (p-Cresol)	0.96	-	-	-	-	-
11	GUAIA-01	2-Methoxyphenol (Guaiacol)	2.89	-	-	-	-	-
12	COMP12	2-Hydroxy-2-cyclopenten-1-one	0.57	-	-	-	-	-
13	DIMET-01	1,3-Dimethoxybenzene	0,35	-	-	-	-	-
14	3:4-X-01	3,4-Dimethylphenol	0.43	-	-	-	-	-
15	4:8-D-01	4,8-Dimethyl-1-nonanol	0.33	-	-	-	-	-
16	4-MET-01	2-Methoxy-4-Methylphenol	1.95	-	-	-	-	-
17	PHENO-02	4-N-Propylphenol	0.31	-	-	-	-	-
18	3-MET-02	3-Methoxy-1,2-Benzenediol	1.47	-	-	-	-	-
19	4-ETH-01	p-Ethylguaiacol	1.99	-	-	-	-	-
20	4-ETH-02	Vinilguaiacol	4.12	-	-	-	-	-
21	SYRIN-01	2,6-Dimethoxyphenol (Syringol)	11.84	-	-	-	-	-
22	4-ALL-01	Eugenol	2.15	-	-	-	-	-

23	4-PRO-01	2-Methoxy-4-Propyl-Phenol	1.13	-	-	-	-	-
24	VANIL-01	2-Methoxy-4-Formylphenol (Vanillin)	1.60	-	-	-	-	-
25	(E)-I-01	Isoeugenol	14.97	-	-	-	-	-
26	COMP26	Isoeugenylmethylether	0.76	-	-	-	-	-
27	ETHYL-01	Ethylvanillin	1.57	-	-	-	-	-
28	ACETO-01	Acetovanillone	1.46	-	-	-	-	0.02
29	COMP29	3,4,5-Trimethoxytoluene	2.95	-	-	-	-	-
30	COMP30	1-(4-Hydroxy-3-Methoxyphenyl) -2-propanone	0.63	-	-	-	-	-
31	COMP31	3,4-Dimethoxyacetophenone	11.55	-	-	-	-	-
32	COMP32	2,6-Dimethoxy-4-(2-Propenyl)- Phenol	4.50	-	-	-	-	-
33	SYRIN-02	Syringaldehyde	6.08	-	-	-	1.00	-
34	4-ACE-01	Acetosyringone	12.05	-	-	-	-	0.98
35	N-HEX-01	n-Hexane	-	10.00	90,00	10.00	-	-

It is possible to observe that the SYRIN-02 component was successfully obtained by extraction. The other components followed the next steps of the process, being the solvent N-HEX-01, having a recovery of 90%, and thus being returned to the process through the recycle stream. The other components of the bio-oil were directed to the next distillation columns, obtaining through this process the compound 4-ACE-01 with 98% purity. The other unwanted components were removed in chains 8 and 10.

3.1.3. Simulation 3

After inserting the blocks, chains and their respective configurations, it was possible to obtain the Process Flow Diagram of Simulation 3 presented in Figure 3, referring to the refining of bio-oil from sugarcane bagasse.

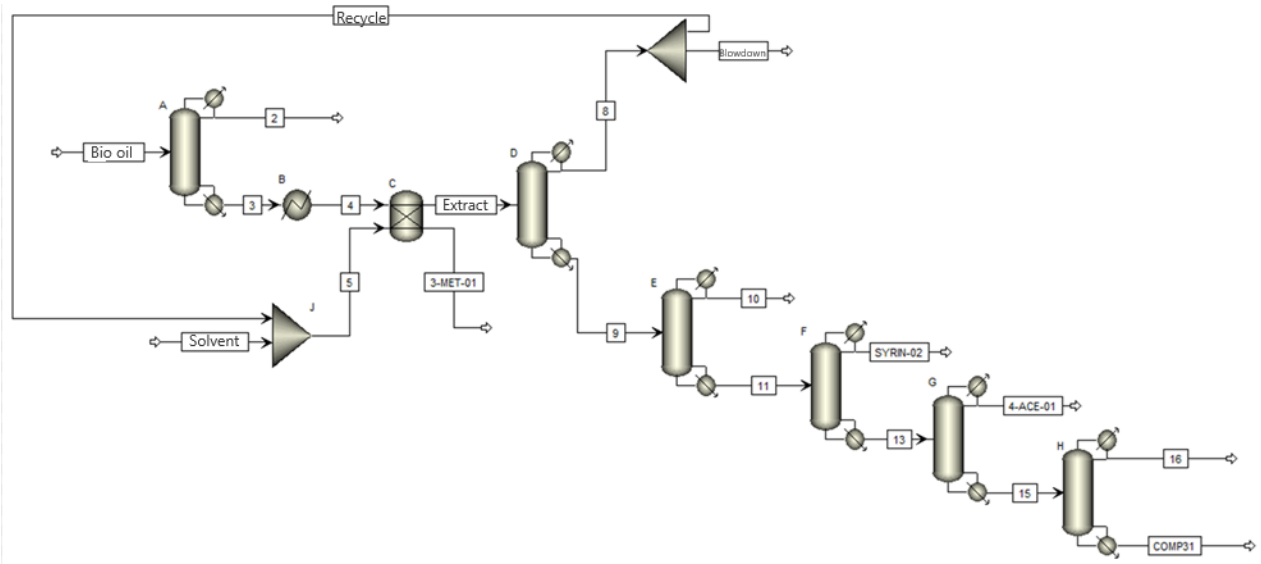

Figure 3 - Simulation 3 Process Flow Diagram (Authors, 2024).

Table 5 describes the unit operations considered in Simulation 3.

Table 5 - Description of the blocks used in Simulation 5 (Authors, 2024).

Name in the simulator	Block ID	Description
RADFRAC	A	Simulates a distillation column to separate bio-oil components that are more volatile than the solvent.
HEATER	B	Simulates a heat exchanger to lower the temperature prior to entry into the extraction column.
SEP	C	Simulates an extraction column to separate the COMP6 component from the others, due to solvent incompatibility.
RADFRAC	D	Simulates a distillation column to separate the solvent from the other products.
RADFRAC	E	Simulate a distillation column to separate a fraction of compounds.
RADFRAC	F	Simulates a distillation column to separate the SYRIN-02 component from the other components.
RADFRAC	G	Simulates a distillation column to separate the 4-ACE-01 component from the other compounds.
RADFRAC	H	Simulates a distillation column to separate the COMP31 component from the other components.
FSPLIT	H	Simulates a separation equipment to separate a fraction of the stream and recover it to the process.
MIXER	I	Simulates a mixer to integrate the recycle stream into the input solvent.

Table 6 shows the results of the currents later the simulation has been performed.

Table 6 - Result of Simulation 3 streams (Authors, 2024).

No. of compounds	Aspen Nomenclature	Compound	Bio oil	Solvent	Reciclo	Blowdown	3-met-01	Syrin-02	4-ace-01	Comp31
			Mass flow (kg/h)							
			100.00	6,00	94.05	5.95	3.14	5.10	5,08	6.38
			Fraction							
1	CARBO-01	Carbon Dioxide	1.23	-	-	-	-	-	-	-
2	PYRUV-01	2-oxo-Propanoic Acid	1.21	-	-	-	-	-	-	-
3	ACETA-01	Acetaldehyde	1.21	-	0.03	-	-	-	-	-
4	ACETI-01	Acetic Acid	1.21	-	-	-	-	-	-	-
5	ACETO-01	1-Hydroxy-2-Propanone	1.21	-	-	-	-	-	-	-
6	2-HYD-01	Monoacetate-1,2-Ethanediol	1.21	-	-	-	-	-	-	-
7	METHY-01	2-oxo-Propanoic Acid Methyl Ester	1.21	-	-	-	-	-	-	-
8	FURFU-02	Furfural	2.69	-	-	-	-	-	-	-
9	FURFU-01	2-Furanemethanol	1.15	-	-	-	-	-	-	-
10	COMP10	2-Hydroxy-2-cyclopenten-1-one	2.75	-	-	-	-	-	-	-
11	METHY-02	Methyl Butanedioic Acid	2.41	-	-	-	-	0.01	-	-
12	COMP12	3-Methyl-2,4(3H,5H)-Furandione	3.20	-	-	-	-	-	-	-
13	3-MET-01	3-Methyl-1,2-Cyclopentanedione	3.14	-	-	-	1.00	-	-	-
14	GUAIA-01	2-Methoxy-Phenol	3.06	-	-	-	-	-	-	-
15	3:4-X-01	3,4-Dimethyl-Phenol	3.00	-	-	-	-	-	-	-
16	4-MET-01	2-Methoxy-4-Methyl-Phenol	3.45	-	-	-	-	-	-	-
17	2:3-D-01	2,3-Dihydro-Benzofuran	3.37	-	-	-	-	-	-	-

18	COMP18	1,4:3,6-Dianhydro-α-D-glucopyranose	1.94	-	-	-	-	-	-	-
19	4-ETH-01	4-Ethyl-2-Methoxy-Phenol	3.85	-	-	-	-	-	-	-
20	4-ETH-02	2-Methoxy-4-Vinylphenol	3.79	-	-	-	-	-	-	-
21	SYRIN-01	2,6-Dimethoxy-Phenol	4,32	-	-	-	-	-	-	-
22	VANIL-01	Vanillin	4.24	-	-	-	-	-	-	-
23	ISOEU-01	2-Methoxy-4-(1-Propenyl)-Isoeugenol Phenol	4.60	-	-	-	-	-	-	-
24	4-PRO-01	2-Methoxy-4-Propyl-Phenol	3.85	-	-	-	-	-	-	-
25	COMP25	3-Methoxy-2,4,6-Trimethyl Phenol	4.24	-	-	-	-	-	-	-
26	LEVOG-01	Levoglucosan	1.68	-	-	-	-	-	-	0.26
27	COMP27	3',5'-Dimethoxyacetophenone	4,63	-	-	-	-	-	-	-
28	SYRIN-02	4-Hydroxy-3,5-Benzaldehyde	5.11	-	-	-	-	0.88	0.12	-
29	COMP29	2,6-Dimethoxy-4-(2-Propenyl)-phenol	5.44	-	-	-	-	-	-	-
30	4-ACE-01	1-(4-Hydroxy-3,5-Dimethoxyphenyl)-Ethanone	5,08	-	-	-	-	0.11	0.88	-
31	COMP31	Desaspidinol	4.69	-	-	-	-	-	-	0.73
32	COMP32	3,5-Dimethoxy-4-Hydroxycinnamaldehyde	5.84	-	-	-	-	-	-	0.01
33	N-HEX-01	n-Hexane	-	6,00	94.02	5.95	-	-	-	-

According to Table 6, it is noted that component 3-MET-01 was successfully obtained by the extraction process. Thus, the stream with the extract was directed to the next step. The solvent was recovered through a distillation column, with 94.02% being directed to the recycle stream that returned to the process. The other components obtained by stream 9, were routed to a sequence of distillation columns, where compounds SYRIN-02, 4-ACE-01 and COMP31 were obtained with 88%, 88% and 73% purity, respectively. The unwanted components were withdrawn at the chains, 10 and 16.

Right away obtaining the results of the three simulations, it was possible to compare the results, evaluating the purity of the compounds obtained. Considering that in the three simulations a product with 100% purity was obtained through extraction, one way to perform a better analysis of the results was through the comparison between Simulations 2 and 3, which used distillation to obtain other compounds. Considering that Simulation 2 had a recovery of only one compound, and this had a considerable purity (name the % purity) compared to the other three compounds obtained in the simulation, it can be observed that the simulation becomes more complex as the goal is to obtain more isolated compounds.

The simulation of the purification process of bio-oil obtained from different biomasses has been little referenced in the literature. Most of the available studies have carried out experimental work to extract compounds from bio-oil (Campos-Franzani *et al*., 2020; Chang *et al*., 2013; Corrêa *et al*., 2021; Krause, 2019; Melo *et al*., 2014; Wang *et al*., 2010; Xu *et al*., 2021).

For a better comparison between the results obtained in the simulations, economic and risk analyses and uncertainties were carried out to better study the three cases, and evaluate the feasibility for the implementation of the projects.

3.2. Results of the economic evaluation with risk and uncertainty analysis

3.2.1. Economic valuation

In Figures 4, 5 and 6 are represented the distributions of the costs of utilities and raw materials for Simulation 1, 2 and 3, respectively.

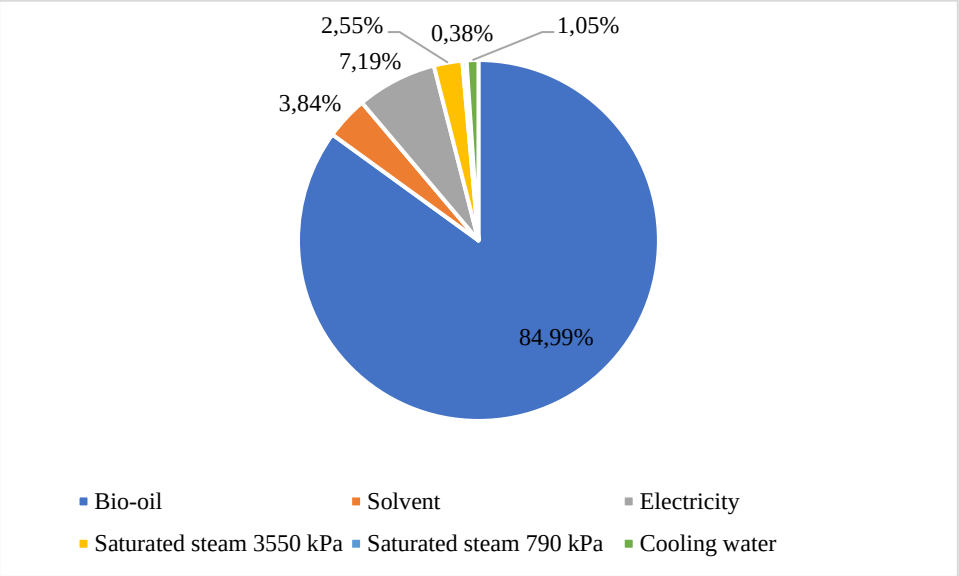

Figure 4 - Distribution of utility costs for Simulation 1 (Authors, 2024).

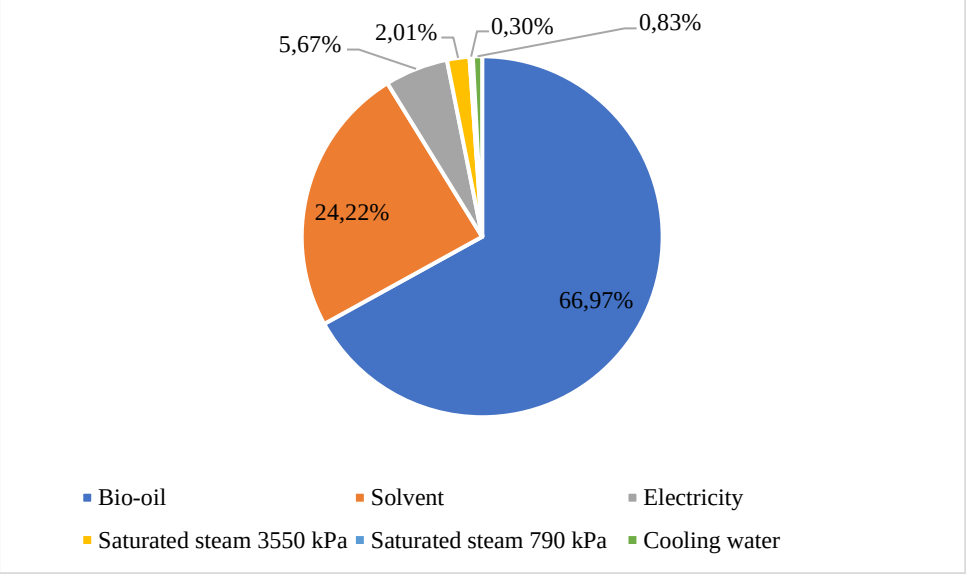

Figure 5 - Distribution of utility costs for Simulation 2 (Authors, 2024).

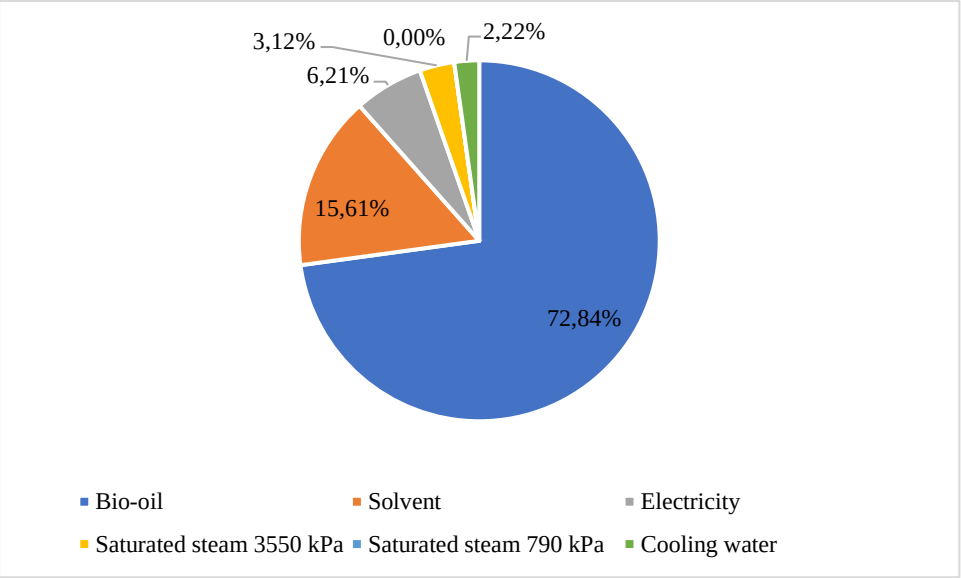

Figure 6 - Distribution of utility costs for Simulation 3 (Authors, 2024).

We can see from the figures that in Simulation 2 we had the highest solvent consumption for the process. This means that there was a lower recycle rate compared to Simulations 1 and 3.

With the investment data and the projection of the cash flows of each evaluated scenario, it was possible to carry out the economic feasibility study. The main parameters evaluated were Internal Rate of Return (IRR), Net Present Value (NPV) and simple payback.

To evaluate the annual profit from the implementation of the industrial plants represented by the simulations, 28% of fees and taxes on annual revenue and 10% of depreciation on the fixed cost of capital were considered.

From the net cash flow value, it was possible to estimate the Net Present Value of the projects during the 24-month period with a Discount Rate (Minimum Attractiveness Rate) of 13.75% per month. NPV can be defined as the algebraic sum of the discounted values of the cash flow associated with it. That is, it is the difference in the present value of revenues minus the present value of costs. The project that presents the NPV greater than zero (positive) is economically viable, being considered the best one that presents the highest NPV (Lopes & Fontes, 2005).

Another important factor for economic evaluation is the Internal Rate of Return (IRR), also called the cash flow discount rate. The IRR is an interest rate implicit in a series of payments (outflows) and receipts (inflows), which discounts a future value or applies the interest factor on the present value (Pereira & Almeida, 2008).

In addition to these factors, the economic feasibility analysis was applied to the Profitability Rate, which relates the sum of the present values and the initial investment, and to the Payback Time, which would be the time spent to recover the amount invested in the process, that is, the higher the IRR, the greater Payback Time and the lower the NPV Table 7 shows the values of the economic parameters evaluated in the three simulations performed.

Table 7 - Results of the economic feasibility analysis (Authors, 2024).

Simulation	1	2	3
Sum of VPs (Months 1 to 24) (R$)	223.90	297.23	859.78
NPV of the Project (R$)	215.63	269.52	773.18
Internal rate of return (TIR) (%)	390.3	154,5	143.0
Profitability rate (%)	27.10	10.73	9.93
Payback Time (years)	0.29	0.74	0.80

The shortest return on invested capital was achieved in the scenario considered in Simulation 1, which corresponds to 0.29 years. However, the three scenarios presented a low payback, less than 01 year. This shows the feasibility of the bio-oil purification process. This quick turnaround time is related to the high price of the product. The values considered in the work were obtained from the literature, however, these values can have considerable oscillations depending on the purity and application of the product.

3.2.2. Risk and uncertainty analysis

Through the results of the economic feasibility study, it was possible to evaluate the risk and uncertainties associated with the implementation of the projects due to the variation in data entry. Using the Monte Carlo technique and with the aid of spreadsheets, it was possible to generate the results of these analyzes. For risk analysis of the projects, the probability distributions are presented, which show the most probable value of the NPV, that is, what is the best range of values to work with given the variations in bio-oil costs. Figures 7 to 9 show the histograms of the distribution for the NPV of the Project referring to the variation of the bio-oil cost of the three Simulations considered.

Within the assumptions adopted, there is an 85% probability that in the scenario considered in Simulation 1 the NPV is between MM R$216.23 and R$216.52, which shows the economic viability of the project, together with a rapid return on the fixed capital invested. In Simulation 2, there is an 86% probability that the NPV is between MM R$269.43 and 269.72. In Simulation 3, NPV is between MMR$774.43 and 775.02, with an 86% probability.

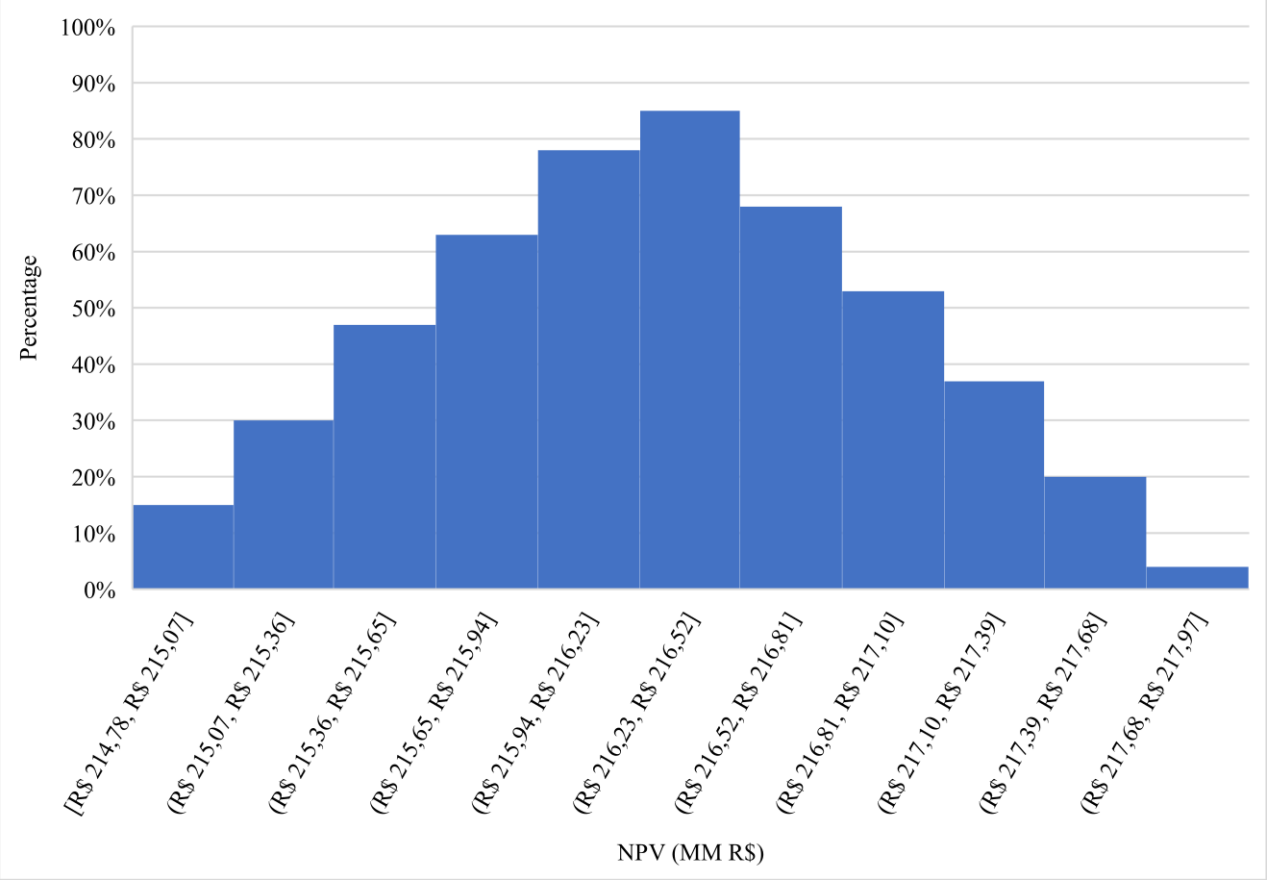

Figure 7 - Probability distribution for the NPV of the Project referring to the variation in the cost of bio-oil (Simulation 1) (Authors, 2024).

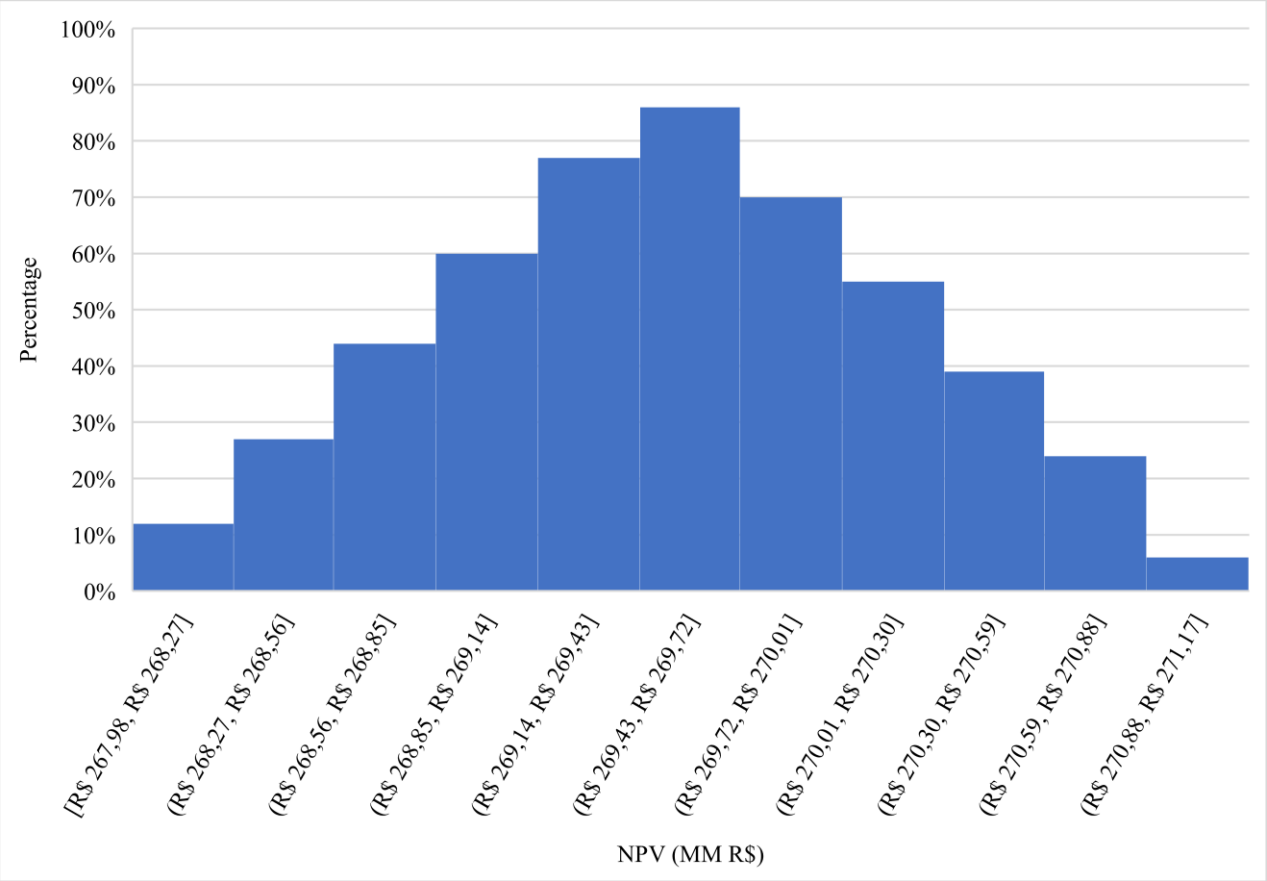

Figure 8 - Probability distribution for the NPV of the Project referring to the variation in the cost of bio-oil (Simulation 2) (Authors, 2024).

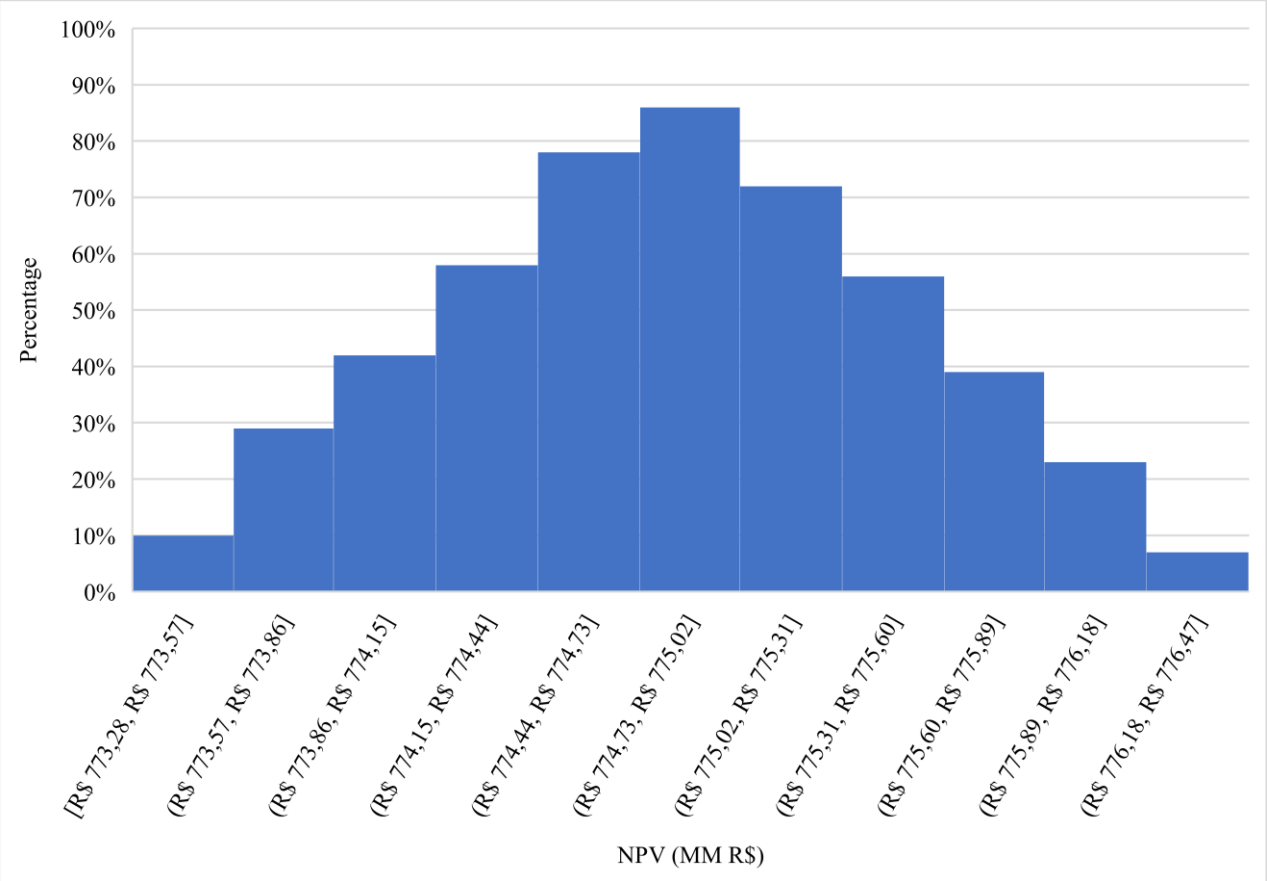

Figure 9 - Probability distribution for the NPV of the Project referring to the variation in the cost of bio-oil (Simulation 3) (Authors, 2024).

4. Conclusion

Based on the evaluation of the results of the simulations, we can infer that the desired products were obtained. The level of purity of the components varies according to their composition, since in some cases it can be challenging to achieve separation due to the similar boiling point relative to other compounds. Consequently, the process can become complex when the goal is to recover different products. After analyzing the economic feasibility of the three scenarios evaluated, it is possible to state that the most advantageous investment is obtained in the scenario considered in Simulation 1 (bio-oil derived from eucalyptus wood). Despite presenting a lower NPV, the project has the best IRR, the highest rate of return and the shortest Payback Time. When evaluating the results of risks and uncertainties for the projects, as well as in the economic analysis, the NPV of Simulation 3 is the most recommended considering a better return on investment and the best probability of the conditions of variation of the cost of bio-oil. The realization of the project can contribute significantly to the area of the chemical and thermochemical industry, since bio-oil is a renewable energy source, derived from raw material often from industrial waste. The compounds present in it have high added value, being used in the manufacture of drugs, chemicals, among others, in addition to contributing to the development, optimization and evaluation of investments in thermochemical processes to obtain such products.

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