

# Simulation of Sugarcane Bagasse Pyrolysis using COCO Simulator

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The search for alternatives to energy derived from fossil sources to decarbonize the environment has been growing in recent years. Therefore, the use of waste to generate energy has been a viable alternative. Among the different types of processes used to transform biomass into energy, pyrolysis, a thermochemical process, stands out for its process versatility and diversity of products for energy applications. This process consists of the thermal decomposition of the organic matrix of the biomass in the absence of oxygen or with a substoichiometric amount of air to avoid combustion, which can produce bio-oil, biochar, and gaseous products. In this context, kinetic parameters obtained from the literature on thermal degradation of biomass were used to evaluate the behaviour of the operating conditions of the process, aiming to obtain optimal product distributions. For this purpose, the COCO (Cape-Open to Cape-Open) simulator with CSTR (Continuous Stirred-Tank Reactor) reactor was used. For these evaluations, parametric studies were performed regarding temperature. The characterization of sugarcane bagasse was crucial for data entry into the simulator, providing real data on the raw material. Thus, proximate, ultimate, and biochemical analyses were performed. The simulation of this process covers the main stages: biomass drying, pyrolysis process, and products separation – biochar, bio-oil, and combustible gases. With fast pyrolysis operating conditions (500 °C), it was possible to obtain the expected yield of liquid products (more than 58 %) in the process.

## 1. Introduction

Biofuels, or fuels derived from biomass, are important alternatives for reducing greenhouse gas emissions, combating global warming (Rial, 2024) and contributing to the global energy supply (Miranda *et al.*, 2019). Considering the available raw materials, the biomass produced by sugar and alcohol plants (sugarcane bagasse) has received significant attention due to its abundance and environmental sustainability, in addition to its great potential for efficient energy generation (Ajala *et al.*, 2021). Brazil is the world's largest producer of sugarcane, producing around 677 million tons of sugarcane in 2024/2025 harvest (CONAB, 2025). However, this large production has generated a high amount of bagasse. Part of the bagasse can be reused as fuel in boilers (Cavalcanti; Carvalho; Silva, 2020) or to produce second-generation bioethanol (Moonsamy *et al.*, 2022). However, the unused part generates a residue that is difficult to control, which can cause negative environmental impacts. Thus, different ways to produce biofuels from biomass have been studied (Kan; Strezov; Evans, 2016). Among these, pyrolysis has received considerable interest due to its ability to efficiently convert lignocellulosic biomass through thermal decomposition (Yogalakshmi *et al.*, 2022). This process consists of the thermal decomposition of the organic matrix of the biomass in the absence of oxygen or a substoichiometric amount of combustion, which can simultaneously produce products in the liquid (tar – bio-oil), solid (coal – biochar) and gaseous (mainly syngas – CO and H<sub>2</sub>) states (Miranda *et al.*, 2021).

Sugarcane bagasse is a fibrous residue consisting of cellulose (32–45 %), hemicelluloses (20–32 %), lignin (17–32 %), ash (1.0–9.0 %) and some extractives (Arni, 2018). These components are randomly scattered throughout the cell wall of the biomass. Cellulose ( $C_6H_{10}O_5$ )<sub>n</sub> is the main component of biomass, and the one most observed in the cell wall of the residue (Miranda *et al.*, 2019; Shabbirahmed *et al.*, 2022). Hemicellulose ( $C_5H_8O_4$ )<sub>m</sub> thermal decomposition occurs in a temperature range between 220 and 315 °C (Yogalakshmi *et al.*, 2022). Lignin [ $C_9H_{10}O_3(OCH_3)_{0.9-1.7}$ ]<sub>x</sub> is the component that provides rigidity, since it has a complex chain of aromatic alcohols (Nanda *et al.*, 2014). Lignin decomposed over a wide temperature range, from 140 to 600 °C, presenting a peak intensity at approximately 380 °C (Stefanidis *et al.*, 2014).

Process simulations are fundamental tools in the design and optimization of chemical processes. Among the many benefits of simulations, economic analysis and the assessment of susceptibility to changes in system variables can be highlighted (Zalazar-Garcia *et al.*, 2022). The COCO simulator is sequential simulation software that operates under steady-state circumstances. This simulator allows modification of the operating variables established through the CAPE standard (Zalazar-Garcia *et al.*, 2022). The fact that the COCO simulator is open software (which does not generate costs for the user) makes it an interesting application tool. Using free simulation software as a tool for simulating chemical processes is encouraging, as it opens possibilities for conducting research in this field in locations where paid software is not available. While existing literature frequently relies on paid software, which can limit access and study replicability, choosing open-source software democratizes knowledge and expands research opportunities. Furthermore, by demonstrating the effectiveness of free software in obtaining precise and reliable results, this study significantly contributes to the recognition of accessible solutions within the academic and professional community, allowing researchers from different regions and institutions to access the same tools, reducing financial barriers. It is also important to highlight that, despite its limitations, COCO software, like other free tools, has an engaged community that continuously contributes to improvements and functionality expansion. Thus, several authors have used this simulator to investigate pyrolysis and biowaste management systems. Tangsathikulchai, Punsuwan, and Weerachanchai (2019) carried out pyrolysis studies with five different biomasses using a kinetic approach. Zalazar-Garcia *et al.* (2022) studied the pyrolysis of 12 types of biowaste at temperatures of 673, 773, and 873 K to indicate the corresponding performance: product yield, CO<sub>2</sub> emission, energy and water consumption through the simulation process. Although other studies have used COCO to simulate biomass pyrolysis, the way they conduct the simulation and insert the biomass differs from the approach taken in this work. Zalazar-Garcia *et al.* (2022) introduce biomass using chemical formulas, meaning that the number of carbon (C), hydrogen (H), and oxygen (O) atoms in the empirical formula of the biowaste is calculated based on ultimate analysis. To simulate, the biomass is decomposed into its main elements: C, O, and H, with each reaction producing a single product. In the present study, the biomass was modeled as being composed of three main macromolecules: cellulose, hemicellulose, and lignin, according to its biochemical analysis. Multiple reactions, based on the work of Humbird *et al.* (2017) and Ranzi *et al.* (2008), were used to represent the thermal degradation of all components, generating various products. Ranzi *et al.* (2008) was one of the pioneers in the kinetic modeling of lignocellulosic biomass pyrolysis and remains one of the most widely used and referenced models in the literature for predicting the behaviour of this process, and the other authors have been improving them, especially Humbird *et al.* (2017). This approach is applicable to various biomasses, as the model is sensitive to biomass composition. In fact, other studies (Motta *et al.*, 2023) have already applied this model to different types of biomasses, demonstrating its variability according to biomass composition. Tangsathikulchai, Punsuwan, and Weerachanchai (2019) employed a similar approach to Zalazar-Garcia *et al.* (2022), using a single chemical formula to represent the biomass, where the subscripts correlate with the percentage of elements present in the tested biomasses. In their work, however, a single reaction was simulated to produce all products. Moliner *et al.* (2018) also studied the biomass gasification process in the same simulator. Thus, this work studies the solid phase pyrolysis process in a CSTR reactor using the COCO simulator, using sugarcane bagasse as biomass. In this context, kinetic parameters obtained from the literature on thermal degradation of biomass were used, which proposes a kinetic reaction model for the thermochemical process, with the aim of predicting the yields and distribution of products.

## 2. Methodology

The methodology used in this study is divided into two fundamental stages: the characterization of sugarcane bagasse and the computational simulation of the pyrolysis process using this biomass as raw material. The sugarcane bagasse used in this work was characterized in its main lignocellulosic components and by proximate analysis focused on moisture content for the simulation. After characterization, simulations of the pyrolysis process were performed using the COCO simulator and its tools. This step aims to simulate the thermochemical process, observe the behaviour of the biomass, and predict the distribution of the products (biochar, bio-oil, and non-condensable gases). At the beginning of the simulation, the lignocellulosic components (unconventional) –

cellulose, hemicellulose, and lignin – were inserted into the COCO simulator database. The process flowchart is characterized by three stages (Figure 1): biomass drying, pyrolysis, and products separation.

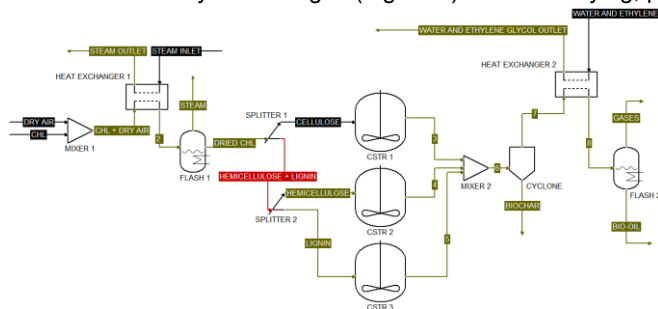


Figure 1: Simulation of the sugarcane bagasse pyrolysis process.

Biomass, represented by the lignocellulosic components (*CHL*), are fed together with *DRY AIR* and then submitted to the *HEAT EXCHANGER 1*, exchanging heat with the *STEAM INLET* entering at 105 °C. The dry biomass (*DRIED CHL*) is separated from the water *STEAM* using the flash separator (*FLASH 1*). In the sequence, *DRIED CHL* goes to *SPLITTER 1*, and it is separated into *CELLULOSE* and *HEMICELLULOSE + LIGNIN*, which also goes through another *SPLITTER 2*, and it is separated into *HEMICELLULOSE* and *LIGNIN*. After this separation, the components are inserted into their respective reactors (cellulose – *CSTR 1*, hemicellulose – *CSTR 2*, and lignin – *CSTR 3*). For each lignocellulosic component there is a set of specific reactions from Humbird *et al.* (2017) (Figure 2), producing the pyrolysis products. The chemical reactions and their respective reaction rates are fed into the simulator.

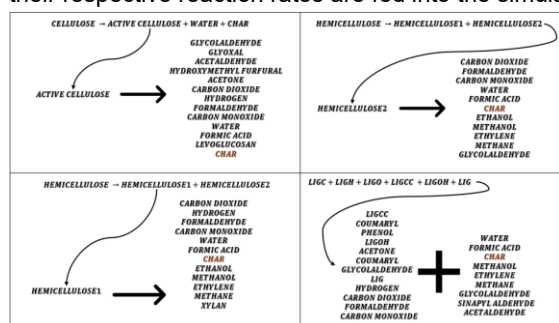


Figure 2: Scheme of reactions of the lignocellulosic components of pyrolysis process and their products (based on Humbird *et al.* (2017)).

The reaction rates implemented in the reactors are represented as follows:  $r = k \cdot e^{\frac{E_a}{RT}} \cdot C$ , where  $r$  is the reaction rate ( $\text{mol}/\text{m}^3\text{s}$ ),  $k$  the constant rate ( $1/\text{s}$ ),  $E_a$  the activation energy ( $\text{J}/\text{molK}$ ),  $R$  the ideal gas constant ( $8.314 \text{ J}/\text{molK}$ ),  $T$  the temperature ( $\text{K}$ ), and  $C$  is the component concentration ( $\text{mol}/\text{m}^3$ ). There are four cellulose reactions, five hemicellulose reactions, and nine lignin reactions, which were all added to the *CSTR 1*, *CSTR 2*, and *CSTR 3* reactors, respectively. In the simulator, kinetic reactions were conducted especially in the solid phase, since this simulator prevents solid components from participating in reactions in the vapor or liquid phase. Thus, solid-only components are compounds that can only occur in the solid phase (COCO HELP, 2025). Furthermore, the *CSTR* reactor is single-phase, allowing reactions to occur only in one phase. Using the *CSTR* reactor was necessary to allow a viable kinetic evaluation within the available tools due to the software's limitations in not performing kinetic assessments in other reactors, even though real pyrolysis does not actually occur in this reactor type. Other studies (Motta *et al.*, 2023) have also used this reactor type to simulate pyrolysis, even in Aspen Plus, to ensure that the kinetic evaluation could be properly conducted. After the reactors, the *MIXER 2* mixes all products from the reactors. Then, in the separation stage, a *CYCLONE* was used to separate the solid products from the gaseous products. The gaseous products enter into the counterflow *HEAT EXCHANGER 2*, exchanging heat with water with ethylene glycol stream at 5 °C to reduce the temperature of this stream. Then, this stream is fed into a condenser, represented by *FLASH 2*, which separates the bio-oil from the combustible gases. Table 1 briefly presents a description of the unit operations applied in the simulation. This study evaluates the yields of pyrolysis products at different temperatures, as the primary focus of this work was to assess the applicability of free software in predicting the impact of temperature variation on the pyrolysis products of sugarcane bagasse. Although pyrolysis yields depend on multiple parameters (e.g., heating rate, residence time, particle size), only temperature variation was explored, as simulators are unable to predict changes in heating rate or residence time. To evaluate the impact of particle size, it would be necessary to use Aspen Plus software.

Table 1: COCO simulator unit operations used in the simulation.

Unit Operation	Definition
Mixer	Mix two or more inlet streams into a single outlet
Heat exchanger	Transfer heat from a hot to a cold stream
Flash type separator	Allows separation of the input stream into vapor and remaining phases
Cyclone	Split compounds between two phases (solid and gas) into predefined fractions
CSTR Reactor	Single-phase mixed reactor for equilibrium and kinetic reactions

### 3. Results and Discussions

Figure 3 shows the behaviour of the different compounds formed during the cellulose pyrolysis process, as a function of the temperature of reactor *CSTR 1*. It shows that cellulose is almost completely consumed at around 360 °C. Then, after that, some compounds began to be formed with more emphasis, such as water, carbon monoxide and dioxide, acetone, formaldehyde, biochar, glycolaldehyde, glyoxal, hydroxymethylfurfural, and levoglucosan, being the most prominent and the compound with the highest yield derived from cellulose pyrolysis, as expected, with yields ranging from 20 to 60 % (Shen *et al.*, 2015). This behaviour is characteristic of primary pyrolysis reactions, such as decomposition and polymerization (Figure 2).

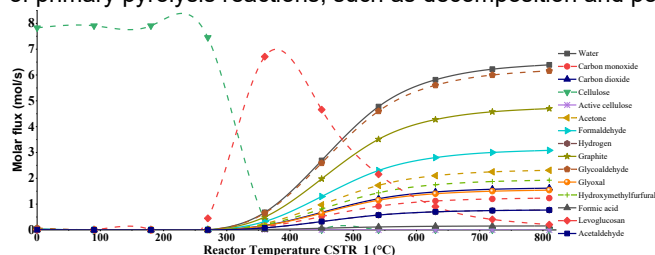


Figure 3: Cellulose pyrolysis products.

Throughout the process, a significant increase in water, glyoxal, biochar, and formaldehyde can be observed, especially after 450 °C. The production of levoglucosan presents a remarkable behaviour, reaching its peak at around 360 °C, agreeing with the work of Zhang *et al.* (2021), in which the highest production of levoglucosan occurred around 300 °C, and in Ranzi *et al.* (2008), where its production peak was approximately 400 °C, yielding 65 % yield of this stream, agreeing with the literature on the range that can be produced. This high production is due to depolymerization and rupture of 1,4-glycosidic bonds, under conditions of high temperatures and prolonged times (Yogalakshmi *et al.*, 2022). However, this percentage may vary depending on the specific conditions of the pyrolysis process, such as temperature, as can be seen that after the peak of production on 360 °C, if higher temperatures would be used, would reduce its production, reaction time, and the type of biomass used (Itabaiana Junior *et al.*, 2020). As the fast pyrolysis temperature occurs at 500 °C, its yield is not the highest, reaching around 14 %. In relation to the other products, constant growth can be observed over the temperature. Acetone, hydroxymethylfurfural, carbon dioxide and monoxide, acetaldehyde, and acid formic reach less than 10 % each of them after 360 to 800 °C. Figure 4 shows the behaviour of the different compounds formed during the hemicellulose pyrolysis process, as a function of the temperature of reactor *CSTR 2*.

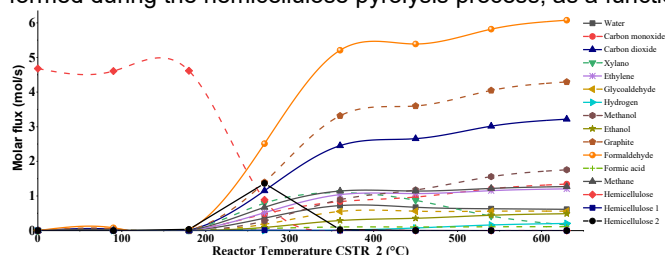


Figure 4: Pyrolysis products of hemicellulose.

Hemicellulose also decomposes completely at around 360 °C. *Hemicellulose 2* is also formed, with its highest peak at 270 °C and complete decomposition at 360 °C, and *Hemicellulose 1* barely appears in these products. The main product formed in this reactor is formaldehyde (around 29 %). Biochar (20 %) and carbon dioxide (15 %) are the other two products that stand out after formaldehyde in this reactor. Regarding the other products formed, they would increase their yields gradually as the temperature increases, but their concentrations are low. Figure 5 illustrates the behaviour of the different compounds formed throughout the lignin pyrolysis process, as a function of the temperature of reactor *CSTR 3*. The predominant formation of biochar (50 %) can be seen regardless of the temperature after 270 to 800 °C, standing out in relation to the other products, as expected since lignin pyrolysis at low to moderate temperatures (< 700 °C) results in the formation of permanent gases,

in addition to condensable tars/bio-oil that contain several low and high molecular weight phenolic compounds, and also generates a solid residue as biochar (Faravelli *et al.*, 2010).

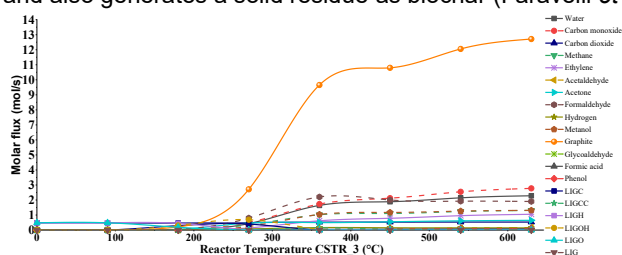


Figure 5: Lignin pyrolysis products.

Also, high biochar production is caused by the fact that lignin has very stable aromatic rings and a high carbon content (Patwardhan; Brown; Shanks, 2011). The other components have yields in this reactor lower than 10 %, emphasizing carbon monoxide, water, formaldehyde, methanol, ethylene, acetone, and others with low prominence. Considering the process, this simulation of the pyrolysis process yielded 9 % of biochar, 58 % of bio-oil and 31 % of combustible gases, agreeing with the range of biomass fast pyrolysis, reported in the literature (Tangsathitkulchai; Punsuwan; Weerachanchai, 2019), specially for gases and liquids. Solids yield did not agree due to the lignin content in the sugarcane bagasse, which is lower when compared to the literature. In summary, the findings highlight the importance of precise temperature control and the inherent properties of cellulose, hemicellulose, and lignin in optimizing pyrolysis yields, offering valuable insights for future biomass conversion processes. Thus, after all these evaluations, for 9500 kg/h at 500 °C, 8.8 % biochar, 58.5 % bio-oil, and 30.8 % gas were obtained. These findings agree with simulation works (Humbird *et al.*, 2017), and experimental works, such as Jamilatun *et al.* (2025), in terms of gases and liquids, Ferreira *et al.* (2025) and Parihar *et al.* (2007), in terms of gases, demonstrating the applicability of this simulator, even with the limitations.

#### 4. Conclusions

Despite the considerations made so that the COCO simulator could simulate this complex process, it was possible to simulate the pyrolysis process of sugarcane bagasse, being able to evaluate how the behaviour of its main products would be, thus obtaining guidance on how to execute in relation to the temperature ranges used. The analysis of the cellulose pyrolysis process revealed that around 360 °C, cellulose is almost entirely consumed, and after that, various compounds begin to form prominently, in which aligns with the continuous breakdown of cellulose and formation of these by-products. Levoglucosan stands out as the most prominent compound, with high yields in this stream (reaching up to 21 %), showcasing its significance in the pyrolysis process. For instance, at the fast pyrolysis temperature of 500 °C, the yield of levoglucosan is lower (around 10 %), highlighting the importance of controlling process parameters to optimize product yields. The findings align with existing literature and provide a comprehensive understanding of the thermal decomposition behaviour of cellulose. Also, in CSTR 2 demonstrates that both cellulose and hemicellulose decompose entirely at around 360 °C, indicating as a crucial temperature for the efficient breakdown of these biomass components, aligning with existing literature and providing valuable insights for optimizing pyrolysis conditions to maximize the production of key compounds (formaldehyde, biochar, and levoglucosan). This work emphasizes the significant role of lignin's chemical properties in determining the yield of biochar and other products during pyrolysis. The findings align with existing literature and provide valuable insights for optimizing pyrolysis conditions to maximize the production of desired compounds such as biochar, bio-oil, and combustible gases. By understanding the behaviour of each component during pyrolysis, it is better optimized processes to maximize desired yields, contributing to advancements in biofuel production and material science. Ultimately, these insights pave the way for more efficient and environmentally friendly applications of biomass in various industries. Given the above, in addition to evaluating a complete thermal degradation process and producing various products through pyrolysis, this study, using free software, was able to conduct simulations like those performed with Aspen Plus, a paid software used for chemical process simulation. By incorporating all reactions and reaction rates of the main macromolecules present in lignocellulosic biomass, this approach provided a broader perspective and allowed for the verification of a wider range of molecules being produced according to the ongoing thermal degradation. No significant impacts from the solid-phase reaction constraints in the COCO simulator were observed on the accuracy of the results, as the same behaviour could be visualized in other simulations using different software. Although this study focused on the technical simulation results in COCO, the industrial feasibility of pyrolysis was not directly addressed. However, the software has the potential for adaptations that would allow the inclusion of industrial parameters, making it possible to predict large-scale operational behaviours. Implementing these modifications would require adjustments to thermodynamic and kinetic models, as well as experimental validation, but could significantly contribute to the practical application of the process.

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