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INVESTIGATING THE ECONOMIC POTENTIAL OF ENZYMATIC BIOSURFACTANT SYNTHESIS

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ABSTRACT

This work aimed to evaluate the economic viability of producing sugar fatty esters, specifically xylose fatty acid esters, through enzymatic biosurfactant synthesis. Sugar esters are surfactants widely used in the cosmetics, food, and pharmaceutical industries due to their biodegradable, odorless, non-irritating, and non-toxic properties. The global market for these products is projected to expand significantly, driven by increasing demand for natural and biodegradable products. A notable challenge in this synthesis is the solubility of sugars in non-polar organic solvents. In this context, this work proposed using eutectic deep solvent (DES), which are advantageous due to their non-toxicity, biodegradability, and ability to act as solvents and substrates in an anhydrous reaction medium. The process involves a novel approach where xylose and choline chloride are mixed and heated to form a liquid phase, followed by adding oleic acid and the enzyme Novozyme 435 (a commercial immobilized lipase B from *Candida antarctica*) for the esterification reaction. The economic potential of this method was assessed through modeling and simulation, considering mass and energy balances to determine the cost-effectiveness of the production process. Preliminary economic analysis indicated a minimum biosurfactant selling price (MBSP) of $15.8/kg, a value below of those reported in the literature, indicating that the process proposed in this work is promising.

Keywords: Sugar esters. Fatty acids. Biosurfactant. Enzymatic process.

1. INTRODUCTION

Fatty acid sugar esters, or simply sugar esters (SEs), are molecules made up of sugars (polar head) linked to fatty acids (apolar tail) via ester bonds[1-4]. Since SEs are non-anionic surfactants, having properties such as biodegradable, odorless, non-irritating, and non-toxic, they can be highly applicable in the cosmetics, food, and pharmaceutical industries. Given their extensive applicability and the growing global demand for biodegradable and natural products, it is expected that the SEs market will grow from US$ 76 million (data from 2020)[5] to US$ 120 million over the next decade[4].

Esters of five-carbon sugars, such as xylose esters, have the potential to be more sustainable once xylose can be obtained from lignocellulosic wastes generated in biorefineries or second-generation ethanol facilities[6-9].

SEs can be produced by enzymatic esterification, catalyzed by lipases, using oleic acid as acyl donar and xylose as acyl acceptor, for example. However, a great challenge for that is solubilize sugars in non-polar organic solvents, which are commonly used as cosolvents in the synthesis[9-12]. Considering this, a new generation of solvents, known as eutectic deep solvents (DES), has been proposed as a promising alternative to the traditional organic solvents[11-13]. DES have several advantages, including non-toxicity, biodegradability, non-inflammability, and non-volatility[14-15]. Furthermore, the DES formed by sugars, which act as donors of hydrogen bonds, can be used simultaneously as solvents and substrates for the reaction, allowing the use of an anhydrous reaction medium containing sugars and fatty acids, which in turn facilitates the catalysis of esterification by lipases[12,14-17]. Although promising, every proposed experimental process must be investigated regarding economic return to evaluate it for industrial-scale production. Therefore, this study aimed to investigate the economic potential of using an eutectic solvent to produce xylose fatty acid esters.

2. MATERIAL & METHODS

The enzymatic process proposed consisted of using xylose and oleic acid as reagents, Novozyme 435 (immobilized lipase) as a biocatalyst, and choline chloride as a solvent in the xylose oleate production (biosurfactant ester). As can be seen in Figure 1, xylose and choline chloride enter in a mixing tank in a 1:1 molar ratio at 90ºC for approximately one hour, both in a solid phase, to liquefy the components. At the exit of the tank, now in the liquid phase, are added oleic acid is added for a molar ratio of 1:5 (xylose: oleic acid), immobilized lipase to reach a ~2% load ($m_{enzyme}/m_{oleic\ acid}$), and molecular sieve to the 1.4 % ($m_{molecular\ sieve}/m_{oleic\ acid}$) into the reactor. Then, the reaction is conducted at 60ºC for 24 hours. Next, the reaction medium leaves the reactor and passes through a filter to remove the molecular sieve and the immobilized enzyme (both have different sizes). Finally, the reaction medium containing the xylose oleate product leaves the process. It should be noted here that the immobilized enzyme could be recycled 10 times.

Modeling and simulation were based on mass and energy balances[18]. The cost of equipment (C_P) is given from Equation 1, where K_i (i=1,3) are specific constants, and A is the area, volume, or diameter. Equation 2 is applied to calculate the modular costs (C_M), with F being the modular factor for each piece of equipment[19].

$$C_P = K_1 + K_2(A) + K_3((A)) \quad (1)$$

$$C_M = C_P \cdot F \quad (2)$$

Location and time are corrected by Equations 3 and 4 (L is the location factor and I is the price index for each time), and the total cost of the plant is given by Equation 5[19].

$$C_L = C_M \cdot L \quad (3)$$

$$C_2 = C_1 \left(\frac{I_2}{I_1}\right) \quad (4)$$

$$C_T = 1.18 \sum_{i=1}^{n} C_{Mi} \quad (5)$$

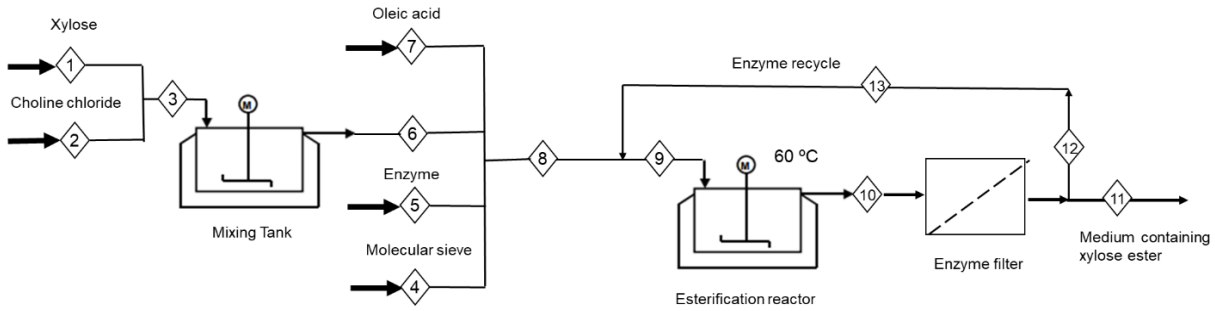
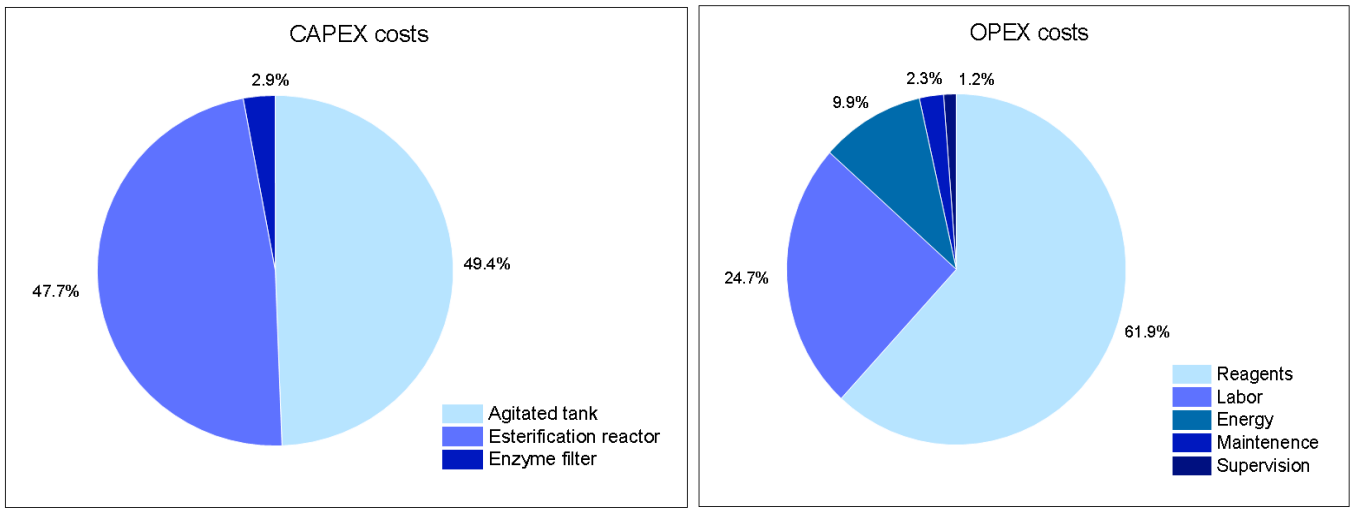


Figure 1 Process diagram for simulation of xylose ester.

3. RESULTS & DISCUSSION

The plant's operating base was 10 kmol/h of xylose being consumed and 10 kmol/h of solvent, with ~3000 kg/h of mass entering the process in the agitated tank. The 24-hour mass conversion of oleic acid was 85%. The agitated tank where solvent and xylose are mixed and changed from solid to liquid phase consumes 266.175 kW, while the esterification reactor requires 2392.75 kW.

The plant installation costs (CAPEX), indicated in Figure 2a, present a balance between the agitated tank and the esterification reactor, while the enzyme filter represents the minor portion. Figure 2b indicates operational costs, with reagents being the most significant portion, followed by the labor, energy, maintenance, and supervision. Without purification processes, the minimum biosurfactant selling price (MBSP) of xylose ester was $15.8/ kg. The MBSP obtained in this word is lower than those previously reported by biosurfactants produced by microbial fermentation, for example, sophorolipid (US$ 20/kg; 90% w/w)[20], glycolipopeptide (€ 570/kg; 110g/L)[21], and rhamnolipids (US$ 60/kg; 60% w/w)[22]. On the other hand, xylose ester enzymatically produced using tert-butanol as cosolvent indicated a MBSP of US$ 72.37/kg (86% w/w)[19]. In addition to MBSP obtained, a cost of approximately US$5/kg must be added for purification steps to find a product with purity similar to sophorolipid, for example.



(a) **(b)**

Figure 2 CAPEX and OPEX costs.

Table 1 Energy spent in the process.

Equipamento	Energia
Agitated tank	266.175 kW
Esterification reactor	2392.75 kW

4. CONCLUSION

An enzymatic process for producing xylose esters (biosurfactants) using oleic acid and xylose as reagents, chlorine chloride as a deep eutectic solvent, and Novozyme 435 as an immobilized enzyme was modelled and simulated. Preliminary economic analysis indicated a MBPS of $15.8/kg, a value lower than previously reported in the literature, indicating that the proposed process is promising.

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