Simulation of a biorefinery process from the organic fraction of municipal solid waste generated in Mexico City

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Abstract

BACKGROUND: In this work a biorefinery process was designed and simulated in Aspen Plus® V.10 for production of biogas, bioethanol and biofertilizer from the Organic Fraction of Municipal Solid Waste (OFMSW) generated in Mexico City (CDMX). The process consists of five stages: 1) anaerobic digestion, 2) acid hydrolysis, 3) simultaneous saccharification and co-fermentation, 4) conventional distillation, and 5) dehydration by extractive distillation. Stirred tank and stoichiometric reactors were used for the anaerobic biodigester simulation, while stoichiometric reactors were employed for simulation of the acid hydrolysis, and simultaneous saccharification and co-fermentation.

RESULTS: The overall results of the simulated process show that it is possible to obtain 149.6 Tons of Biogas, 41.9 Tons of Biofertilizer and 19.7 Tons of Bioethanol from 1000 Tons of OFMSW processed daily, which is equivalent to a total yield of 0.21 Ton Bioproducts/Ton OFMSW or 0.947 Ton Bioproducts/Ton Volatile Solids contained in the OFMSW.

CONCLUSIONS: The conceptual design and simulation of the biorefinery process presented in this work indicates that it is technically feasible to obtain 3 different bioproducts from the OFMSW generated in CDMX. Computer aided process design will allow progress towards the circular economy where biorefineries will play a leading role.

Keywords: Biorefinery simulation, OFMSW, Bioproducts, Bioprocess synthesis.

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INTRODUCTION

It is estimated that world population will reach 10.4 billion by the year 2100, with 68-70% living in cities.[1] It is estimated that this population will generate 3.4 billion Tons of Municipal Solid Waste (MSW).[2] Organic Fraction of Municipal Solid Waste (OFMSW) is a mixture of food waste, from kitchens, residences, restaurants, cafeterias, factory canteens, markets, and vegetable waste from parks and gardens.[3] Various studies have determined that OFMSW constitutes 40-60% of the total MSW generated in different regions, therefore OFMSW has great potential to be used as raw material in the production of biofuels and other valuable bioproducts. Several works have explored viable and cost-effective process options.[4-8]

An average of 120,128 Tons of MSW are generated daily in the country of Mexico.[9] In particular, CDMX generates 13,149 Tons of MSW per day, of which 50% are organic residues.[10] Due to the saturation of its landfills, CDMX exports daily more than 60% of its residues to other states (Mexico and Morelos) with the associated expenses for transportation and land rental which reach 167 million dollars annually.[11]

Biorefineries are essential for the circular economy because they will allow us to obtain added-value products from our residues.[12-13] In the anaerobic biorefinery, Anaerobic Digestion (AD) which is a mature technology for MSW treatment, serves as the centerpiece for the transformation of easily biodegradable organic matter such as food waste into biogas, and as pretreatment for poorly biodegradable compounds such as cellulose, which can be further processed to other value-added bioproducts.[14]

Implementation of biorefinery processes based on Lignocellulosic Biomass (LB), has gained great importance.[15] Replacing current products from oil refineries with renewable bioproducts is vital to reduce the carbon footprint of the chemical industry and the development of a global bioeconomy.[16] Some researchers have analyzed the potential and challenges currently faced by LB biorefineries. These biorefineries can contribute significantly to rural development, job creation, waste reduction and energy diversification, but face high production costs, low conversion efficiencies, immature technologies, logistical problems and variability in raw material composition.[17-19] Because this wide variability in biomass composition based on its source, type, and recalcitrant level, there is no standard method for bioconversion of LB. [20-21] Particularly, the pretreatment stage is the most critical, influential and expensive stage of lignocellulosic bioethanol.[22] Another point to reduce the cost of the process is the development of new enzymes that are more economical for saccharification. Large-scale production of biofuels and biochemicals using LB requires overcoming the various obstacles encountered, and for this purpose computer-aided process design allows the feasibility analysis of different process configurations.

Operational strategies and parameters optimized at laboratory scale generally fail to show a similar level of efficiency in pilot or demonstration scale operations.[23-24] The design of viable biorefineries at commercial scale will require the combination of techno-economic models, technological innovations, life cycle assessments, cost or risk analysis, and of course, simulation and optimization of operations.[25-26]

Process simulation allows the evaluation of different scenarios with acceptable degrees of approximation and in short response times that allow rapid decision-making without compromising high economic resources. The objective of this study was the synthesis and simulation in Aspen Plus® V.10. of a biorefinery process to take advantage of 1000 Tons per day of OFMSW generated in CDMX. In this first study, the simulation and analysis of an anaerobic biorefinery process is presented to analyze its technical and economic viability. In a second study, different configurations of the process will be analyzed to direct production to specific bioproducts.

MATERIALS AND METHODS

OFMSW characterization

Campuzano y González-Martínez[27] reported the chemical and bromatological average compositions of OFMSW from different cities in the world. Specific compositions for OFMSW from CDMX are summarized in Tables 1 and 2.

Table 1. Average chemical composition for OFMSW from CDMX[27]

Humidity (%)	TS (%)	VS (%)	VS/TS (%)
70.3	29.7	22.3	75.1

TS: Total solids, VS: Volatile Solids

Table 2. Average bromatological composition for OFMSW from CDMX[27]

			Crude fiber (39.5%)		
Fat/oil (%)	Protein (%)	Total carbohydrates (%)	Lignin (%)	Cellulose (%)	Hemicellulose (%)
17.5	15.2	52.9	13.3	21.1	5.1

All values are in percent of Volatile Solids (% VS)

Table 1 shows that 75.1% of TS in the OFMSW are VS, which can be used for biogas and bioethanol production while Table 2 indicates in turn that the main components of VS are carbohydrates, followed by fatty components, and proteins.

Representative OFMSW constituents were obtained from Rajendran et al.[28] who previously developed the simulation of an OFMSW biodigestion process, which was the starting point for our study. For simulation purposes, carbohydrates were represented as cellulose, hemicellulose, starch, and dextrose (free sugars); starch and free sugars were determined from the difference between total carbohydrates and crude fiber (13.4%); lipids were introduced as triolein, tripalmitate, palmito-olein and palmito-linolein in equivalent mass fractions; soluble and insoluble (keratin) proteins were incorporated as pseudocomponents. Other compounds such as starch or palmito-olein, are not present in the Aspen Plus® V.10 databases, so they are represented by equivalent compounds. Ashes (TS-VS) and lignin were considered inert in the proposed process, which is predominantly biological.[29] Table 3 summarizes the average OFMSW composition from CDMX considering its representative constituents and chemical and bromatological characteristics.

Table 3. OFMSW compounds used for simulation purposes

Component	Aspen Plus® Representation	Condensed formula	Mass fraction
Carbohydrates	Cellulose	$(C_6H_{12}O_6)_n$	0.0471
	Hemicellulose	$C_5H_8O_4$	0.0114
	Dextrose	$C_6H_{12}O_6$	0.0234
	Starch	$(C_6H_{12}O_6)_n$	0.0381
Proteins	Protein (Pseudo)	$C_{13}H_{25}O_7N_3S$	0.0212
	Keratin (Pseudo)	$C_{4.39}H_8NO_{2.1}$	0.0127
Lipids	Triolein	$C_{57}H_{104}O_6$	0.0098
	Tripalmitate	$C_{51}H_{98}O_6$	0.0098
	SN-1-Palmito-2-Olein	$C_{37}H_{70}O_5$-1	0.0098
	SN-1-Palmito-2-Linolein	$C_{37}H_{68}O_5$-1	0.0098
Lignin	Lignin	Inert (Pseudo)	0.0300
Ashes	Ashes	Inert (Pseudo)	0.0739
Humidity	Water	H_2O	0.7030
		Total:	1.0000

Component specifications and thermodynamical method

Most of the components used in the simulation were taken as conventional from the extensive Aspen Plus® database; soluble protein, keratin and inert were defined as pseudocomponents due to their complex structure and the fact that they are not found in the software database, and other compounds (biomass and polysaccharides) were defined as solids. Non-Random Two-Liquid (NRTL) model was considered as the property method because it can describe vapor-liquid (VL) and liquid-liquid (LL) equilibria of strongly non-ideal solutions, correlating and calculating the mole fractions and activity coefficients of different compounds.[30]

Biorefinery process conceptual design

In this work, the development of a complete biological process was sought, which base is the use of anaerobic digestion (AD) as the heart of the biorefinery.[14] The choice of AD technology was made because it is a low-complex process, friendly to the environment, with high efficiency and quite economical in terms of capital and operating costs.[31] The conceptual design of the biorefinery resulted in five stages, as shown in Figure 1.

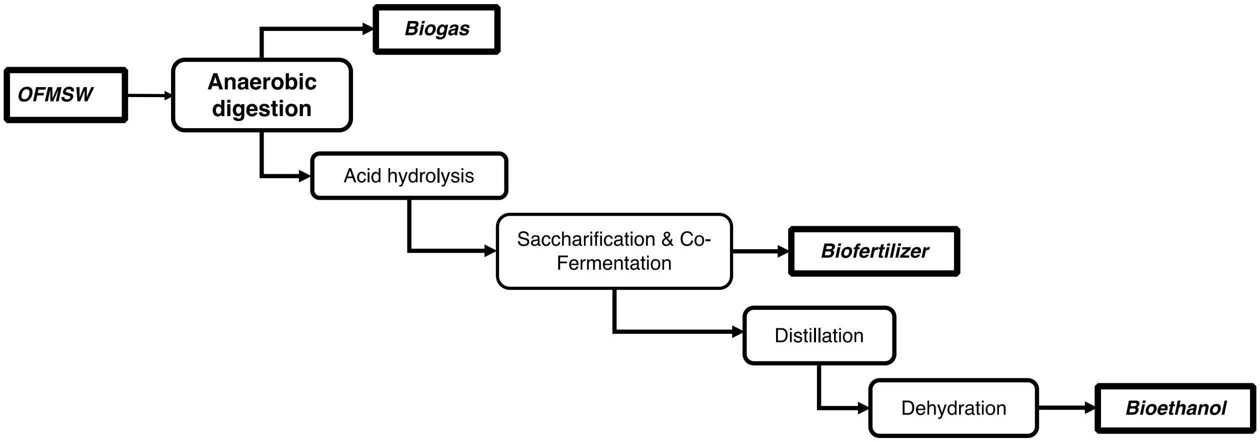

Figure 1. Conceptual design of biorefinery process

The process begins with AD to break down the OFMSW and produce biogas. The resulting solid fibers and the effluent are sent to subsequent stages of pretreatment by hydrolysis, simultaneous saccharification and co-fermentation of sugars (pentoses and hexoses) to produce bioethanol, and finally distillation and dehydration to obtain anhydrous bioethanol. The biofertilizer is obtained as a by-product of the sugar fermentation stage.

Process simulation

The Process Flow Diagram (PFD) was built using Aspen Plus® V10 software considering rigorous kinetics (CSTR) for the AD,[28] and stoichiometric reactors for acid hydrolysis, and simultaneous saccharification and co-fermentation. All stoichiometric reactions were obtained from previous studies developed by Angelidaki et al. (1999),[32] Rajendran et al. (2014),[28] and the US National Renewable Energy Laboratory (NREL) for lignocellulosic bioethanol.[33-35] The biorefinery´s PFD is shown in Figure 2.

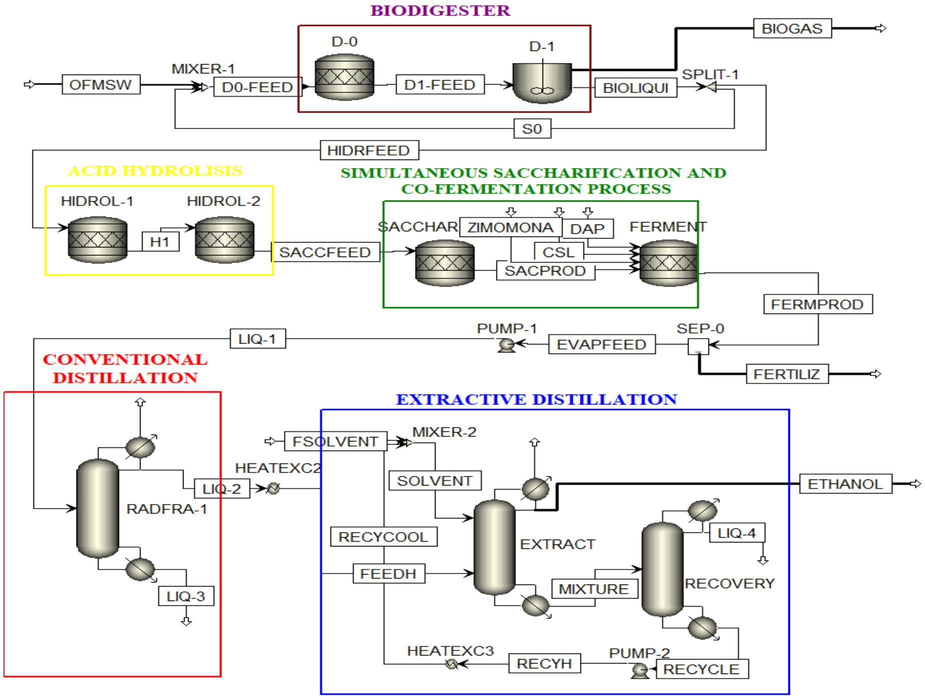

Figure 2. PFD of the anaerobic biorefinery simulated in Aspen Plus® V10

Process simulation was designed to process 1,000 Ton/day of OFMSW (Figure 2), taking the average composition for CDMX provided in Table 3.

Anaerobic digestion

OFMSW was first fed to the anaerobic biodigester where biogas and digestate streams are obtained (Figure 2). For AD simulation a previous model from Rajendran et al.[28] was adapted for OFMSW from CDMX, modifying its chemical and bromatological composition. The feed flow rate and the volume of the anaerobic digester were also increased for industrial production. The model of Rajendran et al.[28] is based on the ADM 1 model developed by the International Water Association.[36] The ADM1 model was developed based on previous models, and is considered the most complete and widely applied. In this model, both biochemical and physicochemical processes are included. The reactions and kinetic parameters used by ADM1 are supported by multiple experimental works, including Angelidaki et al.[32] and Henze et al.[37] In this work, two reactors were used at the same pressure and thermophilic temperature conditions (1 atm and 328.15 K).[38] The first reactor is stoichiometric (D-0) and it includes 13 reactions that hydrolyze carbohydrates, proteins, and lipids into sugars, amino acids, alcohols and short-chain carboxylic acids, respectively. In the second reactor (D-1) which is kinetic (RCSTR), 34 reactions were considered including amino acid degradation, acidogenic, acetogenic and methanogenic with a residence time of 15 days. [28] All stoichiometric and kinetic reactions of both reactors (reported in Appendix A) and their parameters were taken from Rajendran et al. [28] Fortran calculators were used in D-1 including the effect of inhibitions, kinetic rates, production of ammonia, reactor volume, charging rate and retention time on reaction rates.

Simulation of the bioethanol process

In AD, most of the easily biodegradable compounds (proteins, fatty compounds, starch and free sugars) are reduced to biogas, while the recalcitrant compounds (lignocellulosic) are partially or not digested. Therefore, a second section of the process was proposed to obtain lignocellulosic bioethanol from the digestate. This section includes acid hydrolysis, simultaneous saccharification and co-fermentation, distillation and dehydration by extractive distillation. Furthermore, the biomass grown in the co-fermentation stage is recovered as a byproduct that can be used as biofertilizer.

Acid hydrolysis

Digestate hydrolysis was simulated using two stoichiometric reactors (Figure 2), both operating at the same pressure and temperature conditions (12.1 atm and 463.15 K).[39] The first reactor (HIDROL-1) uses diluted acid (H_2SO_4, 2% v/v) to break lignin and convert hemicellulose into shorter chain polysaccharides such as: mannans, xylans, glucans, galactans and arabinans in the same proportions. The second reactor (HIDROL-2) converts the polysaccharides chains of the first reactor into oligosaccharides, and the latter into their corresponding monosaccharides: mannose, xylose, glucose, galactose and arabinose. Hydrolysis reactions also produce soluble lignin, acetic acid, biodegradation products mainly furfural and hydroxymethylfurfural (HMF), and TAR (a final breakdown compound of carbohydrate polymers). A total of 26 reactions (see Appendix A) were used for chemical hydrolysis; stoichiometry and fractional conversions were obtained from NREL reports.[33-35]

Simultaneous Saccharification and Co-Fermentation process (SSCF)

For SSCF simulation two stoichiometric reactors were employed, both operating at 1 atm and 314 K (Figure 2). In the first reactor (SACCHAR), 6 reactions were included for enzymatic hydrolysis of cellulose and the remaining starch into cellobiose and glucose. In the second reactor (FERMENT), 24 reactions (see Appendix A) were included representing the co-fermentation of pentoses and hexoses to produce bioethanol adding *Zymomonas mobilis* (genetically modified to ferment both hexoses and pentoses), as well as Corn Fermented Liquor (CSL) and Di-Ammonium Phosphate (DAP) as nutrients in the culture medium. Feeding specifications of ZYMOMONA, CSL and DAP streams are shown in Table 4. Stoichiometry and fractional conversions in both reactors were adopted from Aden et al.[33], and Woolye et al.[35]

Table 4. Feed specification for FERMENT reactor inlet streams

	Current		
Specification	**ZYMOMONA**	**CSL**	**DAP**
Temperature (K)	314.15	293.15	293.15
Pressure (atm)	1	1	1
Flow (Ton/day)	3.6	2.04	1.2
Composition	0.5 H_2O 0.5 $C_5H_7NO_2$	1.0 CSL	1.0 DAP

Biofertilizer recovery

At the exit of FERMENT reactor, a split separator (SEP-0) was placed to obtain the biofertilizer (Figure 2). The specifications of split fractions at the outlet of the FERTILIZ stream were 0.03 water, 0.935 biomass ($C_5H_7NO_2$) and 0.005 inert, in order to obtain a humidity percentage between 40 and 60%, which are optimal levels of a biofertilizer or compost.[10]

Conventional distillation

The simulation of this stage was carried out using a RadFrac column (RADFRA-1). This column concentrates the alcoholic broth to near the azeotropic point (Figure 2). The liquid stream (LIQ-1), coming from SEP-0, feeds the RADFRA-1 column whose specifications were obtained from Nabgan et al.[40] by modifying the condenser from total to partial one. The operating conditions are shown in Table 5.

Table 5. RADFRA-1 operating conditions

Specifications	**RADFRA-1**
Function	Rectification column
Model	RadFrac
Stages	18
Condenser	Liquid-Vapor-Partial
Re-boiler	Boiler
Specified boiling ratio	0.228
Specified reflux ratio	2.3
Temperature (K)	Upper stage/condenser 300 Lower stage/boiler 384.99
Pressure (atm)	1.5

Extractive distillation (dehydration)

Due to the formation of an azeotropic mixture between bioethanol and water an extractive distillation was proposed to remove the remaining water from the LIQ-2 effluent stream. This stage was simulated using two RadFrac columns to obtain pure ethanol. The first column (EXTRACT) is fed by the streams FEEDH and SOLVENT, where FEEDH comes from the conventional distillation and SOLVENT is a mixture of the streams FSOLVENT and RECYCOOL. FSOLVENT contains pure glycerol (1 atm and 353.15 K), while the RECYCOOL stream contains the recovered glycerol from the second column (RECOVERY). Design specifications for extractive distillation were taken from Gil et al.[41] and adapted to the conditions of this process. Table 6 presents the operating conditions of columns EXTRACT and RECOVERY.

Table 6. Operating conditions of the columns used in extractive distillation

	Equipment:	
Specifications	**EXTRACT**	**RECOVERY**
Function	Purification column	Recovery column
Model	RadFrac	RadFrac
Stages	11	11
Condenser	Partial-Vapor-Liquid	Total
Re-boiler	Boiler	Boiler
Distillate rate (kmol/h)	18.24	8
Specified reflux ratio	0.35	0.25
Temperature (K)	Upper stage/condenser	
	327.5	356.24
	Lower stage/kettle	
	500.36	517.04
Pressure (atm)	0.5	0.2

RESULTS AND DISCUSSION

To analyze the results of the simulation, the yields obtained from the process are first expressed in terms of the OFMSW that enters the anaerobic digestion, and subsequently in terms of the Biodegradable Volatile Solids (BVS) that enter the rest of the equipment. The results are shown below and discussed for each stage of the biorefinery.

Anaerobic digestion

Starting from a feeding of 1000 Ton/day of OFMSW with composition described in Tables 1 and 2, 297 Ton/day of TS and 223 Ton/day of VS are obtained, the difference (74 Ton/day) corresponds to the Fixed Solids (FS), which were included with lignin (30 Ton/day) as inert material. This means that there are only 193 Ton/day of Biodegradable Volatile Solids (BVS) that can be used to obtain bioproducts. The anaerobic biodigester converts BVS into biogas with high methane content and poorly biodegradable compounds in digestate which can be additionally processed as biofertilizer and for bioethanol production.

The obtained biogas mass flow was 149.6 Ton/day which means a biogas yield of 0.15 Ton Biogas/Ton OFMSW or 0.77 Ton Biogas/Ton BVS. Therefore, 77.5% of BVS contained in the OFMSW were transformed into biogas. Moreover, developing a mass balance for the BVS in the biodigester, it is found that only 104.35 Ton/day are consumed, and 88.75 Ton/day are contained in the digestate, expressing the yield per Consumed BVS (CBVS) the value obtained is 1.43 Ton Biogas/Ton CBVS. Mol fractions of methane and CO_2 in biogas stream were 0.6156 and 0.2144, with mass flows of 65.58 and 62.65 Ton /day, respectively. These 65.58 Ton/day of methane are equivalent to 9.164×10^7 normal liters per day (NL/day), so the methane production yield obtained is 411 NL/kg VS. Campuzano and González-Martínez,[27] report an average methane yield of 415±137.7 NL/ kg VS obtained from anaerobic digestion experiments using OFMSW from 43 cities in 22 different countries, particularly the value reported in particular for an experiment in CDMX is 545 NL/kg VS.

Therefore, the AD simulation is capable of reproducing both methane yield and composition of biogas that traditionally contains 50-80% methane and 20-50% CO_2.[42-43] Biogas produced in this process can be used to generate heat and electricity.

The liquid digestate stream called BIOLIQUI (HIDRFEED) contains mainly water and inert (including lignin), followed by $C_5H_7NO_2$ (biomass) and bioethanol, which are recovered in later stages as other bioproducts. As previously mentioned, this stream has a mass flow of 88.75 Ton BVS/day, and contains mainly cellulose (CELLULOS), xylose

(XYLOSE), starch (STARCH), insoluble protein (KERATIN), soluble protein (PROTEIN) and hemicellulose (HEMECELL) entering the next hydrolysis stage. The bioethanol produced in the AD (12.03 Ton/day) is equivalent to a mass fraction in the digestate of 1.4%.

Acid Hydrolysis

The objective of this stage is to solubilize mainly the sugars of hemicellulose, composed of pentoses (arabinose and xylose) and hexoses (glucose, mannose and galactose), and partially cellulose (composed of glucose). The feeding current was named HIDRFEED and has the same conditions as the BIOLIQUI current. The results of the simulation at this stage showed that the hydrolysis percentages of cellulose and hemicellulose were 8.4 and 100% respectively, the last percentage being an operating condition. It was determined that 9.88 Ton/day of fermentable monosaccharides are obtained in this stage mainly from hemicellulose (with xylose as the main component 8.01 Ton /day). These 9.88 Ton/day of fermentable sugars correspond to a yield of 0.11 kg fermentable sugar /kg BVS.

The obtained concentration of fermentable sugars was 6.8 g/L. Hafid et al.[44] reported concentrations of 33.9 g/L and 41.2 g/L of sugars when hydrolyzing OFMSW with 1.5% HCl and 1.0% H_2SO_4 (90 °C, 3 h) respectively. It is evident that sugar concentration of this work is lower than values reported by Hafid et al.[44]; this is explained by considering the previous use of easily biodegradable sugars during anaerobic digestion, which were incorporated into the biogas.

Simultaneous saccharification and co-fermentation

The simulation results for the saccharification stage (SACCHAR) indicated that hydrolysis percentages were 95.2% and 100% for cellulose and starch, respectively. This doubled the concentration of fermentable sugars obtained in hydrolysis passing from 9.88 to 19.79 Ton/day, which corresponds to a yield of 0.22 kg fermentable sugar/kg BVS. Bioethanol production in the co-fermenter was 9.01 Ton/day obtaining a yield of 0.46 kg bioethanol/kg fermentable sugar. This value is similar to the theoretical (stoichiometric) yield of 0.51 kg bioethanol/kg glucose reported by Nabgan et al.[40] for corn starch glucose. Fermentation also produces CO_2, mass flow of CO_2 was doubled at the co-fermenter effluent, passing from 7.43 to 15.62 Ton/day.

Biofertilizer recovery

At this stage, the solids formed predominantly by biomass ($C_5H_7NO_2$) generated during the stages of anaerobic digestion and fermentation were separated to be recovered as biofertilizer. 41.9 Ton/day of biofertilizer were obtained which composition is 47% water and 53% solids, biomass was 83.6% of these solids and the rest inert material (lignin, ashes and salts). The EVAPFEED stream containing the liquid phase from fermentation broth passes to the bioethanol recovery process. This stream only conserves 12.8 Ton/day (6.6%) of the original BVS presented in the OFMSW, the rest has been transformed into biogas, biofertilizer (BioFert), bioethanol (BioEtOH) and various other compounds throughout the process.

Conventional distillation

The bioethanol mass flow in the distillation column decreased from 21.04 Ton /day in the influent (LIQ-1) to 19.87 Ton/day in the effluent (LIQ-2), but bioethanol mass fraction was increased from 2.6 to 92%. Likewise, the water mass fraction was reduced from 78.9 to 7.37%. Due to the formation of the azeotropic mixture between bioethanol and water an extractive distillation was proposed to remove the remaining water (1.59 Ton /day) from the LIQ-2 effluent stream.

Extractive distillation (bioethanol dehydration)

The LIQ-2 current with a purity of 92% of bioethanol enters the extractive distillation that consists of two distillation columns in series, pure glycerol is used as solvent to break the water-bioethanol azeotrope. The second column recovers the glycerol from the bottom, which is recirculated back to the first column. This reduces the mass flow of the solvent feed stream (FSOLVENT) to 11.05 Ton/day. The FEEDH stream has the same composition as the LIQ-2 stream, but its temperature increases from 26.8 to 77 °C when passing through a heat exchanger (HEATEXC2). SOLVENT stream is in turn formed by the FSOLVENT stream (with fresh glycerol) and the stream (RECYCLE) that recirculates the glycerol from the second column. Bioethanol mass flow in the final stream (ETHANOL) slightly decreased when compared to the input stream (FEEDH), passing from 19.87 to 19.62 Ton /day, while mass fraction was increased from 92 to 99.6% obtaining anhydrous bioethanol that can be used as biofuel.

Global results (biorefinery)

The anaerobic biorefinery produced 149.6 Ton of biogas, 41.9 Ton of biofertilizer and 19.7 Ton of bioethanol daily, which would be equivalent to a global yield of bioproducts of 0.21 Ton Bioproducts/Ton OFMSW or 0.947 Ton Bioproducts/Ton VS. Therefore 94.7% of the volatile solids presents in the OFMSW were integrated into bioproducts. The biogas stream had a composition that is within the standards to be considered as biogas (0.60 of CH_4 and 0.23 of CO_2).[42-43] Moreover, the percentage of humidity of the biofertilizer is in accordance with those reported in the solid waste inventory of Mexico City (47% humidity and 53% organic matter).[10] Finally, the yield and the purity of the bioethanol were similar to those reported by other authors for fuel bioethanol.[45] The overall results of the process are summarized and compared with experimental values obtained from the literature in Table 7.

Table 7. Global results of bioproduct yields and their comparison with the literature

Bioproducts	Simulation	Literature
Biogas	411 NL/kgVS	545 NL/kgVS [27]
Biofertilizer	47 % Humidity 53 % Organic matter	35 % Humidity [10] 40 % Organic matter [10]
Bioethanol	0.46 kg bioethanol/kg fermentable sugar 99.6% Bioethanol	0.46 kg bioethanol/kg glucose [40] 99.8% Bioethanol [45]

In future work, the process configuration will be modified to create a modular biorefinery where the OFMSW can enter both the bioethanol process and the digestion process, depending on the bioproduct requirements. In this first study we consider that anaerobic biorefinery is an ideal process, since anaerobic digestion is a proven technology for the treatment of OFMSW.

Sensitivity analysis

Although the biorefinery model was developed for the average chemical and bromatological composition of the OFMSW from Mexico City,[27] the effect of varying the VS/TS ratio was analyzed. Campuzano and González-Martínez[27] also report chemical and bromatological compositions of the OFMSW obtained from 44 cities in 22 different countries. From this reference, it was determined that the VS/TS ratio ranges from 43 to 94.9%. To determinate the answer of the simulation to possible variations in SV/ST ratio, two additional simulations were performed maintaining the average humidity, but in the first case adjusting VS/TS ratio to the minimum (43%), and in the second case to the maximum (94.9%). Table 8 presents a summary of the mass flows of bioproducts obtained while Table 9 shows the biogas molar fractions obtained for each scenario (S1, VS/TS = 43%; S2, VS/TS = 75.1%; S3, VS/TS = 94.9%).

Table 8. Mass flows (Ton/day)

	OFMSW	BIOGAS	FERTILIZ	ETHANOL
S1	1000.00	80.12	37.75	11.95
S2	1000.00	149.61	41.90	19.70
S3	1000.00	201.58	46.35	21.28

Table 9. Biogas Mole Fraction

	S1	S2	S3
H_2O	0.1597	0.1522	0.1479
CH_4	0.5904	0.6156	0.6328
CO_2	0.2256	0.2144	0.2041

It can be observed in Table 8 that the mass flows of all bioproducts increase as the VS/TS ratio increases. As expected, the mole fractions of CH_4 and CO_2 increase with increasing VS/TS ratio (Table 9). Therefore, we can conclude that the simulation results are robust.

Economic evaluation of the process

The Aspen Process Economic Analyzer tool was used to estimate capital and annual operating costs, to analyze the economic viability of the process. The results are summarized in Table 10.

Table 10. Economic evaluation of the biorefinery process

Total capital cost (USD)	19,128,700
Total operating cost (USD/Year)	5,062,770
Total utilities cost (USD/Year)	951,242
Equipment cost (USD)	12,818,800
Total installed cost (USD)	17,925,700

It is important to mention that this analysis only included the cost of equipment, electricity, and cooling and heating utilities (cooling water and steam) considered in the default software evaluation. During the economic evaluation all the equipment was correctly mapped, evaluated and sized. The total installed cost was 93.7% of the total capital cost, while the total utilities cost was only 18.79% of the total operating cost.

The cost of the bioethanol separation train was estimated at 5,184,600 USD (40.4% of the total equipment cost), which limits the economic viability of the project due to obtaining only 41.9 tons of this product daily. Therefore, it is proposed as future work to evaluate other process configurations where OFMSW can directly enter bioethanol production. However, the anaerobic biorefinery proposed in this study is currently the most suitable technical option, due to the maturity of anaerobic digestion technology for the OFMSW treatment.[14]

Environmental and energetic aspects of the process

Unlike physicochemical processes for OFMSW treatment such as incineration, pyrolysis, and gasification, biological processes require significantly less energy because they are carried out under mild temperature and pressure conditions. The process proposed in this work is predominantly biological. The main energy consumption occurs in the pretreatment and separation train of the lignocellulosic bioethanol process.[22] The main gaseous emission from the process is CO_2, during the fermentation of sugars, while the main liquid emission (dilute H_2SO_4) is generated during the pretreatment of lignocellulosic biomass. This acid must be neutralized before disposal. In the case of solids, the majority is recovered in the production of biofertilizer. It is clear that a predominantly biological process presents multiple environmental advantages with respect to physicochemical processes, while obtaining products from waste, contributing to the circular economy.

CONCLUSIONS

The average composition of the OFMSW generated in CDMX was obtained from literature in terms of starch, cellulose, hemicellulose, lignin, proteins and fat molecules. This OFMSW composition was used as a starting point for conceptual and basic engineering design of a biorefinery process, considering an anaerobic digester as the core of the process. The main results of the simulation process suggest that obtaining three bioproducts (biogas, biofertilizer and bioethanol) is technically feasible. Of the volatile solids contained in OFMSW, 67.1% were transformed into biogas, 18.8% into biofertilizer, and 8.8% into bioethanol. Computer aided process design will allow progress towards the circular economy where biorefineries will play a leading role. It is important to evaluate different process configurations that allow maximizing the yield of the different bioproducts while minimizing the environmental and energetic impacts of the process. In this first study, the simulation of an anaerobic biorefinery process was implemented to assess its technical and economic feasibility. In a second study, different process configurations will be analyzed to target production of specific bioproducts.

DATA AVAILABILITY STATEMENT

The simulation model is available free of charge at https://lab.anahuac.mx/~jrocha/. The data sources used to feed the model parameters and variables are properly cited in the article.

ACKNOWLEDGMENTS

This work was supported by Universidad Autónoma de Chapingo (institutional support for teaching staff pursuing postgraduate studies), and the scholarship for doctoral studies of Arturo Pérez-Román provided by Universidad Anáhuac México Norte [Centro de Alta Dirección en Ingeniería y Tecnologías (CADIT)].

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APPENDIX A. Model reactions.

Table A.1. Reactions and their conversion fractions in D-0 (Stoichiometric reactor)

Num.	**Component**	**Reaction**	**Reaction advance**
1	Cellulos	Cellulos + Water → Dextrose	0.3
2	Hemecell	Hemecell + Water → 2.5 Aceti-Ac	0.3
3	Tripalm	Tripalm + 3 Water → Glycerol + 3 Palm	0.9
4	Triolein	Triolein + 3 Water → Glycerol + 3 Oleic-Ac	0.9
5	Sn-1--01	Sn-1--01 + 2 Water → Glycerol + Palm + Oleic-Ac	0.9
6	Sn-1--02	Sn-1--02 + 2 Water → Glycerol + Palm + Linoleic	0.9
7	Hemecell	Hemecell + Water → Xylose	0.6
8	Xylose	Xylose → Furfural + 3 Water	0.6
9	Starch	Starch + 7 Water → 7 Dextrose	0.8

10	Cellulos	Cellulos + Water → 2 Ethanol + 2 CO_2	0.5
11	Ethanol	2 Ethanol + CO_2 → 2 Aceti-Ac + Methane	0.7
12	Protein	Protein + 6 Water → 6.5 CO_2 + 6.5 Methane + 3 NH_3 + H_2S	0.9
13	Keratin	Keratin + 0.3337 Water → 0.045 Arginine + 0.048 Aspartic + 0.047 Threonin + 0.172 Serine + 0.074 Glutamic + 0.111 Proline + 0.25 Glycine + 0.047 Alanine + 0.067 Cysteine + 0.074 Valine + 0.07 Leucine + 0.046 Isoleuci + 0.036 Phenylal	0.5

Table A.2. Reactions of the AMINOACI block in D-1 (Kinetic reactor)

Num.	**Component**	**Reaction**	**Kinetic constant**
14	Glycine	Glycine + Hydrogen → Aceti-Ac + H_3N	$1.28E10^{-02}$
15	Threonin	Threonin + Hydrogen → Aceti-Ac + 0.5 Buty-Ac + H_3N	$1.28E10^{-02}$
16	Histidin	Histidin + 4 Water + 0.5 Hydrogen → Formamid + Aceti-Ac + 0.5 Buty-Ac + 2 H_3N + CO_2	$1.28E10^{-02}$
16	Arginine	Arginine + 3 Water + Hydrogen → 0.5 Aceti-Ac + 0.5 Propi-Ac + 0.5 Valer-Ac + 4 H_3N + CO_2	$1.28E10^{-02}$
18	Proline	Proline + Water + Hydrogen → 0.5 Aceti-Ac + 0.5 Propi-Ac + 0.5 Valer-Ac + H_3N	$1.28E10^{-02}$
19	Methioni	Methioni + 2 Water → Propi-Ac + CO_2 + H_3N + Hydrogen + CH_4S	$1.28E10^{-02}$
20	Serine	Serine + Water → Aceti-Ac + H_3N + CO_2 + Hydrogen	$1.28E10^{-02}$
21	Threonin	Threonin + Water → Propi-Ac + H_3N + Hydrogen + CO_2	$1.28E10^{-02}$
22	Aspartic	Aspartic + 2 Water → Aceti-Ac + H_3N + 2 CO_2 + 2 Hydrogen	$1.28E10^{-02}$
23	Glutamic	Glutamic + Water → Aceti-Ac + 0.5 Buty-Ac + H_3N + CO_2	$1.28E10^{-02}$
24	Glutamic	Glutamic + 2 Water → 2 Aceti-Ac + H_3N + CO_2 + Hydrogen	$1.28E10^{-02}$
25	Histidin	Histidin + 5 Water → Formamid + 2 Aceti-Ac + 2 H_3N + CO_2 + 0.5 Hydrogen	$1.28E10^{-02}$
26	Arginine	Arginine + 6 Water → 2 Aceti-Ac + 4 H_3N + 2 CO_2 + 3 Hydrogen	$1.28E10^{-02}$
27	Lysine	Lysine + 2 Water → Aceti-Ac + Buty-Ac + 2 H_3N	$1.28E10^{-02}$
28	Leucine	Leucine + 2 Water → Valer-Ac + H_3N + CO_2 + 2 Hydrogen	$1.28E10^{-02}$
29	Isoleuci	Isoleuci + 2 Water → Valer-Ac + H_3N + CO_2 + 2 Hydrogen	$1.28E10^{-02}$
30	Valine	Valine + 2 Water → Buty-Ac + H_3N + CO_2 + 2 Hydrogen	$1.28E10^{-02}$
31	Phenylal	Phenylal + 2 Water → Benzene + Aceti-Ac + H_3N + CO_2 + Hydrogen	$1.28E10^{-02}$
32	Tyrosine	Tyrosine + 2 Water → Phenol + Aceti-Ac + H_3N + CO_2 + Hydrogen	$1.28E10^{-02}$
33	Tryptoph	Tryptoph + 2 Water → Indole + Aceti-Ac + H_3N + CO_2 + Hydrogen	$1.28E10^{-02}$
34	Glycine	Glycine + 0.5 Water → 0.75 Aceti-Ac + H_3N + 0.5 CO_2	$1.28E10^{-02}$
35	Alanine	Alanine + 2 Water → Aceti-Ac + H_3N + CO_2 + 2 Hydrogen	$1.28E10^{-02}$
36	Cysteine	Cysteine + 2 Water → Aceti-Ac + H_3N + CO_2 + 0.5 Hydrogen + H_2S	$1.28E10^{-02}$

Table A.3. Reactions of the ACIDOGEN block in D-1 (Kinetic reactor)

Num.	**Component**	**Reaction**	**Kinetic constant**
36	Dextrose	Dextrose + 0.1115 H_3N → 0.1115 $C_5H_7NO_2$ + 0.744 Aceti-Ac + 0.5 Propi-Ac + 0.4409 Buty-Ac + 0.6909 CO_2 + 1.0254 Water	$9.54E10^{-03}$

38	Glycerol	Glycerol + 0.04071 H_3N + 0.0291 CO_2 + 0.00005 Hydrogen → 0.04071 $C_5H_7NO_2$ + 0.94185 Propi-Ac + 1.09308 Water	1.01E10^{-02}

Table A.4. Reactions of the ACETOGEN block in D-1 (Kinetic reactor)

Num.	Component	Reaction	Kinetic constant
39	Oleic-ac	Oleic-Ac + 15.2359 Water + 0.482 CO_2 + 0.1701 NH_3 → 0.1701 $C_5H_7NO_2$ + 9.02 Aceti-Ac + 10.0723 Hydrogen	3.64E10^{-12}
40	Propi-01	Propi-01 + 0.06198 NH_3 + 0.314336 Water → 0.06198 $C_5H_7NO_2$ + 0.9345 Aceti-Ac + 0.660412 Methane + 0.160688 CO_2 + 0.000552 Hydrogen	1.95E10^{-07}
41	Isobu-01	Isobu-01 + 0.0653 NH_3 + 0.5543 CO_2 + 0.8038 Water + 0.0006 Hydrogen → 0.0653 $C_5H_7NO_2$ + 1.8909 Aceti-Ac + 0.446 Methane	5.88E10^{-06}
42	Isova-01	Isova-01 + 0.0653 NH_3 + 0.5543 CO_2 + 0.8044 Water → 0.0653 $C_5H_7NO_2$ + 0.8912 Aceti-Ac + Propi-01 + 0.4454 Methane + 0.0006 Hydrogen	3.01E10^{-08}
43	Linoleic	Linoleic + 15.356 Water + 0.482 CO_2 + 0.1701 NH_3 → 0.1701 $C_5H_7NO_2$ + 9.02 Aceti-Ac + 10.0723 Hydrogen	3.64E10^{-12}
44	Palm	Palm + 15.253 Water + 0.482 CO_2 + 0.1701 NH_3 → 0.1701 $C_5H_7NO_2$ + 8.4402 Aceti-Ac + 14.4978 Hydrogen	3.64E10^{-12}

Table A.5. Reactions of the METHAN block in D-1 (Kinetic reactor)

Num.	Component	Reaction	Kinetic constant
45	Aceti-ac	Aceti-Ac + 0.022 H_3N → 0.022 $C_5H_7NO_2$ + 0.945 Methane + 0.066 Water + 0.945 CO_2	2.39E10^{-03}
46	Hydrogen	14.4976 Hydrogen + 3.8334 CO_2 + 0.0836 H_3N → 0.0836 $C_5H_7NO_2$ + 3.4154 Methane + 7.4996 Water	2.39E10^{-03}

Table A.6. Reactions of the H_2 block in D-1 (Kinetic reactor)

Num.	Type	Reaction	Kinetic constant
47	Equilibrium	2 CO_2 + 4 Hydrogen + 0.0836 H_3N ↔ Aceti-Ac + 2 Water	2.39E10^{-03}

Table A.7. Reactions and conversion fractions in HIDROL-1 (Stoichiometric reactor)

Num.	Reaction	Conversion fraction
1	Hemecell + Water → Mannan	0.2
2	Hemecell + Water → Xylan	0.2
3	Hemecell + Water → Glucan	0.2
4	Hemecell + Water → Galactan	0.2
5	Hemecell + Water → Arabinan	0.2

Table A.8. Reactions and conversion fractions in HIDROL-2 (Stoichiometric reactor)

Num.	Reaction	Conversion fraction
6	Mannan → Manolig	0.025
7	Mannan + Water → Mannose	0.925

8	Mannan → HMF + 2 Water	0.05
9	Xylan → Xylolig	0.025
10	Xylan + Water → Xylose	0.925
11	Xylan → Furfural + 2 Water	0.05
12	Glucan → Glucolig	0.025
13	Glucan + Water → Glucose	0.925
14	Glucan → HMF + 2 Water	0.05
15	Galactan → Galaolig	0.025
16	Galactan + Water → Galactos	0.925
17	Galactan → HMF + 2 Water	0.05
18	Arabinan → Arabolig	0.025
19	Arabinan + Water → Arabinos	0.925
20	Arabinan → Furfural + 2 Water	0.05
21	Cellulos → Glucolig	0.007
22	2 Cellulos + Water → Cellobio	0.007
23	Cellulos + Water → Glucose	0.07
24	Acetate → Aceti-Ac	1.0
25	Furfural + 3 Water → TAR	1.0
26	HMF + 3 Water → 1.2 TAR	1.0

Table A.9. Reactions and conversion fractions in SACCHAR (Stoichiometric reactor)

Num.	Reaction	Conversion fraction
1	Cellulos → Glucolig	0.04
2	2 Cellulos + Water → Cellobio	0.012
3	3 Cellulos + Water → Glucose	0.9
4	Cellobio + Water → Glucose	1.0
5	Dextrose → Glucose	1.0
6	Starch + Water → Glucose	1.0

Table A.10. Reactions and conversion fractions in FERMENT (Stoichiometric reactor)

Num.	Reaction	Conversion fraction
1	Glucose → 2 Ethanol + 2 CO_2	0.900
2	Glucose + 0.04696 CSL + 0.018DAP --> 6 Zymo + 2.4 Water	0.073
3	Glucose + 2 Water → 2 Glycerol + O_2	0.004
4	Glucose + 2 CO_2 → 2 Succinic + O_2	0.006
5	Glucose → 3 Aceti-Ac	0.015
6	Glucose → 2 Lacti-Ac	0.002
7	3 Xylose → 5 Ethanol + 5 CO_2	0.8
8	Xylose + 0.03913 CSL + 0.015 DAP --> 5 Zymo + 2 Water	0.126
9	3 Xylose + 5 Water → 5 Glycerol + 2.5 O_2	0.003
10	Xylose + Water --> Xylitol + 0.5 O_2	0.046

11	3 Xylose + 5 CO_2 → 5 Succinic + 2.5 O_2	0.009
12	2 Xylose → 5 Aceti-Ac	0.014
13	3 Xylose → 5 Lacti-Ac	0.002
14	3 Arabinos → 5 Ethanol + 5 CO_2	0.8
15	Arabinos + 0.03913 CSL + 0.015 DAP --> 5 Zymo + 2 Water	0.166
16	3 Arabinos + 5 Water → 5 Glycerol + 2.5 O_2	0.003
17	3 Arabinos + 5 CO_2 → 5 Succinic + 2.5 O_2	0.015
18	2 Arabinos → 5 Aceti-Ac	0.014
19	3 Arabinos → 5 Lacti-Ac	0.002
20	Galactos → 2 Ethanol + 2 CO_2	0.8
21	Galactos + 0.04696 CSL + 0.018 DAP --> 6 Zymo + 2.4 Water	0.166
22	Galactos + 2 Water → 2 Glycerol + O_2	0.003
23	Galactos + 2 CO_2 → 2 Succinic + O_2	0.015
24	Galactos → 3 Aceti-Ac	0.014
25	Galactos → 2 Lacti-Ac	0.002
26	Mannose → 2 Ethanol + 2 CO_2	0.8
27	Mannose + 0.04696 CSL + 0.018 DAP --> 6 Zymo + 2.4 Water	0.166
28	2 Mannose + 4 Water → 4 Glycerol + 2 O_2	0.003
29	3 Mannose + 6 CO_2 → 6 Succinic + 3 O_2	0.015
30	Mannose → 3 Aceti-Ac	0.014
31	Mannose → 2 Lacti-Ac	0.002