Optimization of biogas production through anaerobic digestion of municipal solid waste: a case study in the capital area of Reykjavik, Iceland

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ABSTRACT

BACKGROUND: Biogas is a valuable carbon-free renewable energy source that can be produced from anaerobic digestion of organic waste. Accordingly, biogas production is promoted worldwide in efforts to reduce carbon emissions and optimizing the recovery of resources from waste streams. In this paper the biogas production from bio residues collected in the capital area of Reykjavik was modelled in Aspen Plus v10.

RESULTS: Municipal solid waste, food waste and lignocellulosic biomass were the feedstocks used in this research. 16 scenarios were simulated at thermophilic temperature conditions of 55 ºC. Each scenario accounted for different inlet mass flows, varying the kind of feedstock i.e. municipal solid waste (MSW), food waste (FW), lignocellulosic biomass (LCB), or co-digestion of various feedstocks, using two model approaches: (i) one digestion stage; (ii) two stages coupled in series. Sizing, costing, and environmental aspects were analyzed for all the scenarios. A sensitivity analysis was carried out by changing the substrate concentration and its effect over the methane mass flow. Simulations showed biogas yields measured in mL per gram of volatile solids (VS) in the range of 305.5-406.4 mL/g VS (single-stage approach); and biogas yields ranging from 64.78 to 358.8 mL/g VS (two-stage approach). Maximum methane yields were obtained using LCB as feedstock resulting in 106.0 mL/g VS.

CONCLUSION: From a technical viewpoint the highest biogas yield is obtained when using municipal solid waste whereas optimum calorific value of biogas and electrical power potential is achieved working in co-digestion of various feedstocks.

Keywords: anaerobic digestion, aspen plus, biogas, biomethane, simulation

INTRODUCTION

About 22% of the worldwide primary energy supply is attributed to natural gas. While natural gas is usually produced from fossil sources, it can also be generated from organic waste, through the production of biogas by anaerobic digestion (AD). Biogas which is a mixture of gases (mainly CH_4 and CO_2) has become increasingly important as a renewable energy source in Europe[1] and the entire world.[2] In 2015 the biogas production in the EU accounted for 1.2 billion m[3], to be used either for combined heat and power (CHP) generation or upgraded to produce biomethane ($CH_4 \geq 95$ % v/v), that can be fed in existing natural gas pipelines, after pressurization, or used as vehicle fuel or in fuel cells[3]. In fact, the EU is the largest producer of biomethane, which is mainly used in the transportation sector. Within the bioenergy sector, biogas contributions are planned across all energy sectors: heating, transport and electricity. In this sense, the EU Member States must submit National Renewable Energy Action Plans laying out how they will achieve their binding renewable targets across different energy sectors.[4]

The AD process has many advantages such as low energy consumption, low production of biological solid wastes, the ability to work independently without any feed for long intervals, low nutrient and chemical requirements, high carbon oxygen demand (COD) removal rates, improvement to dewaterability, production of energy gases, and odor-free end products.[5–7] In addition to economic benefits from energy and fuel generation, AD plants provide additional environmental benefits such as a decrease in water, soil and air pollution through emission reductions of greenhouse gas emissions (GHG) and other pollutants.[8]

Most common feedstocks used for AD are: animal manure[9], municipal solid waste (MSW)[10], food waste (FW)[11,12], lignocellulosic biomass (LCB)[13], wastewater[14], sewage sludge[15] or algae [2]. Among them, the most popular is MSW which consists of food waste, yard waste, wood, plastics, papers, metals, leather, rubbers, inert material, and other non-specified components[16]. In recent years anaerobic digestion of MSW has become popular all over the world. Case studies have been described in Mexico[17], the Netherlands[18], Scandinavia[19], South Africa[20], Indonesia[21], Australia, Italy and Spain[22], Brazil[14], to name just a few recent examples. The majority of MSW is generated by households (55-80 %), while only a small portion is generated by commercial or market areas (10-30 %). Accordingly, MSW is typically highly heterogeneous, requiring a sophisticated management of the waste to minimize environmental impacts. Furthermore, the composition of MSW depends on the region, economy, population, and season. Currently, 1.3 billion tons of biowaste are generated per year all over the world and by 2025 this amount will increase to 2.2 billion tons per year[23].

Regarding FW, about 1.3 billion tons of food and one-third of the total global food production is wasted each year, costing the world economy about 750 billion dollars[24]. Organic components of food waste include fruits, vegetables, cooked food waste, meat, etc. Generated during production, handling, storage, processing and consumption[25].

Biomass refers to any type of animal or plant, which can be converted to energy and it can be divided into three categories: residues, standing forests and energy crops. [26] In central and north Europe, AD is widely applied in the agricultural sector. Most of the centralized biogas plants treat manure together with other organic wastes. The annual amount of manure and other biomass treated is about 1.5 million tons per year producing biogas equivalent of about 39 million m^3 CH_4/year.[27]

Rapid population growth, improvement in living standards and urbanization in developing countries are imminent development that calls for a sustainable management of MSW to minimize impacts on the environment[28]. On the other hand, the management of MSW is usually joined with other kinds of materials as FW and lignocellulosic residues. Through adequate MSW and other mixed waste management, biogas can be generated by AD of the organic waste, which can subsequently contribute significantly to the energy sector.[29] The recovery of biogas from this kind of waste is also in-line with the zero-waste objective postulated in circular economy policies. Nevertheless, little is known about the management and optimization of biogas generation from municipal waste in the arctic and sub-arctic environments.

In early 2018 the Icelandic Government published an ambitious Climate Action Plan for the years 2018-2030 intending to become a carbon-neutral country by 2040.[30] The Action Plan postulates two main pillars: (1) to phase out fossil fuels in transport; (2) to increase carbon sequestration in land use by restoration, revegetation and afforestation. To reach fossil-free transportation, the Icelandic government plans to ban new registrations of fossil fuel cars after 2030.[30] Furthermore, recent studies of air quality in the capital area of Reykjavik showed that cars and trucks running on methane emit lower amount of Volatile Organic Compounds (VOC) (500-300 mg.VOC/m^3) in comparison with diesel cars (5000 mg.VOC/m^3).[31,32] In this work, the waste flux and its potential for biogas generation in the subarctic city of Reykjavik, located in southwest Iceland, is modelled, analyzed and optimized.

The present study investigates for the first time the AD process of the bio-residues from the metropolitan area of Reykjavik which mainly consists of MSW, FW and LCB. For this purpose, the Aspen Plus (AP) v10 software was used to simulate different AD conditions and feedstock processing with the aim to optimize the biogas and methane production in the local landfill of SORPA. The study concludes by providing valuable suggestions to the waste company on how to optimize biogas production in Reykjavik.

EXPERIMENTAL

To analyze and optimize biomethane production from MSW, the AP v10 software was used to create 2 AD model approaches simulating a total of 16 scenarios for biogas production in the Reykjavik capital area. The input data were recollected from the local waste company and other governmental agencies in order to simulate realistic conditions of the future biogas plant that will be installed in the Reykjavik area, processing the organic waste fraction. Four AD stages were contemplated in the models: (i) hydrolysis of carbohydrates, proteins and fats into sugars, amino acids and fatty acids respectively; (ii) acidogenesis of such smaller compounds in carbon, acids, alcohols, hydrogen, ammonia and carbon dioxide; (iii) acetogenesis producing acetic acid, carbon dioxide and hydrogen; (iv) and methanogenesis producing biogas.

Biogas yields, methane yields, electrical power potential, calorific biogas value, economic costs or environmental aspects (in terms of CO_2 equivalent) of the 16 proposed AD scenarios were discussed. Total capital costs, operating costs, costs associated with utilities, equipment and installed costs were determined through the aspen plus economy analyzer tool (APEA). Capital costs are fixed costs incurred on construction and equipment, in other words, the total cost needed to bring a project to commercially operable status. Operating costs are associated with the maintenance and administration including direct costs of goods sold from operating expenses. Utility costs is the cost incurred by using electricity, water, heating or waste disposal. Equipment costs include costs of vessels, pipelines and in general all the unit operations used in the plant. Installed costs are the total cost of labor and materials of the facility.

The amount and composition of the digestate was also considered. The digestate, is the main by-product of AD and could be used as soil fertilizer contributing reforestation which is also an objective of the climate Action plan of the Icelandic government.

Bio residue generation and composition

Data of the generated residues of MSW, FW, LCB and the sum of the total bio-residues of the Reykjavik area are represented in Fig. 1. In the last 3 years, SORPA collected more than 11000 t/year of MSW, followed by 8000 t/year of LCB and 1000 t/year of FW. Total bio residues generated from 2016 up to 2019 in tones are shown in Table 1. Average daily inlet flows were introduced into the models. MSW, LCB and FW compositions were taken from the literature.[13,33–35]

Model description

Aspen Plus (AP) is a process simulation software package used in industry to simulate thermodynamic and chemical reactions in industrial processes. AP uses mathematical models to predict the performance of user-defined processes. Two anaerobic digestion (AD) models (i) single-stage AD and (ii) two-stage AD were developed using Aspen Plus v10 to predict the biogas and methane yields among other techno-economic and environmental parameters (Fig. 2a and Fig. 2b).

The single-stage model (Fig. 2a), consists of one stoichiometric reactor where the four AD reactions occur in the same unit following the scheme and extent of reactions published by Nduse and Oladiran[36]: i) hydrolysis, ii) acidogenesis, iii) acetogenesis and iv) methanogenesis. The two-stage AD model (Fig. 2b), consists of one stoichiometric reactor to convert carbohydrates, proteins and fats in sugars, amino acids and fatty acids respectively (hydrolysis reactions); the second reactor is a continuous stirred tank reactor (CSTR) where conversion of such compounds into biogas takes place (acidogenesis, acetogenesis and methanogenesis reactions). Such configuration follows the model of Rajendran.[37] The main difference between two model approaches consist of the reaction scheme (7 reactions in the first model versus 45 reactions in the two-stage AD model). In addition, first model does not contemplate inhibitors or byproducts formation.

Based on the model operating conditions, the thermodynamic model of the Non-Random Two-Liquid model (NRTL) was chosen as the property method. NRTL correlates and calculates the mole fractions and activity coefficients of different compounds and facilitates the liquid and the gas phase in the biogas production. Accordingly, NRTL is the most suitable method for this case study, also supported by the literature for biogas modelling.[26,38–40]

The chemical reactions of the two-stage AD model are described in Table 2. The hydrolysis reactions are in both cases the same. However, in the second model acidogenic, acetogenic and methanogenic reactions in the CSTR are also considered. 7 reactions are contemplated in the first model (Fig. 2a), whereas 33 reactions are contemplated in the second model (Fig. 2b, Table 2) (33,36).

This model does not include the analysis of biogas purification. A compressor in combination with a flash unit was used to ensure final CH_4 concentrations above 95 % v/v, such methane levels are necessary to feed existing natural gas pipelines or be used as vehicle fuels in existing combustion engines.[3] However, there is no reference to the purification phase of this model because this is not the aim of this work and purification was not optimized.

Scenarios

A total of 16 scenarios (operating at varying inlet flow, kind of feedstock or in co-digestion) in two different model approaches (one or two digestion steps in series) have been performed in the last Aspen Plus version v10, as visualized in Fig. 2a and Fig. 2b. All the simulated scenarios are described in Table 3.

As summarized in Table 3, inlet flows vary between 3 t/d up to 323 t/d considering the real and maximum residual streams of SORPA. Co-digestion or in other words combination of all residual streams was also considered.

The selected temperature regime was thermophilic at 55 ºC because AD working in the range of 50 to 65 ºC is the best regime for maximizing biogas production, particularly higher digestion rates in fat-containing materials.[6,41] Therefore, less residence time is needed, and smaller reactors can be used. The only drawback is that higher energy for heating is consume in comparison with mesophilic conditions at 37 ºC.

Validation: theoretical methane yields

Models were validated first theoretically and then by using experimental data from other authors at laboratory, pilot, and industrial scale. Theoretical methane yields at standard temperature and pressure (STP) in terms of mL CH_4 per gram of feedstock. Aspen Plus gives mass fractions of the resulting biogas streams. By using molecular weight is possible to transform mass fractions into moles of cellulose, hemicellulose, protein, or fats. Then is necessary to transform moles of feedstock constituent into moles of biogas constituent (CH_4, CO_2, NH_3 and H_2S). Real moles per constituent were calculated by using conversion factors. Finally, real moles are converted to mL using density of the four aforementioned biogas constituents.

RESULTS AND DISCUSSION

Single-stage stoichiometric AD model approach

Biogas yields, biogas composition in terms of CH_4 and CO_2, purified methane yields, digestate volume flow and electrical power potential of the first eight simulated scenarios are shown in Table 4. Biogas yield of all simulated scenarios are in the range of 305.5 and 406.4 mL/g VS in accordance with yields provided from cow dung (337-567 mL/g VS) and sewage sludge (215-384 mL/g VS) and obtained at laboratory scale under thermophilic conditions by Mohamed et al.[10] Similar results were obtained at farm-scale providing biogas yields of 300 mL/g VS using cow dung and 450 mL/g VS using sheep dung.[42] Best biogas yields in this research were obtained using as raw material

MSW by combination with FW and LCB (co-digestion scenarios), because the quantity of carbohydrates is in these cases higher than the rest of the formulated scenarios.

On the one hand, working with a single feedstock, LCB residue provides the highest methane yields, reaching up to 106.0 mL/g VS (SC3) similar to the methane yields of 139.8 mL/g VS obtained from cattle manure as reported by Sawatdeenarunat et al.[35] Nevertheless, biogas yield reaches a maximum when using MSW (SC1), this is in accordance with the calorific value (CV) of 622,326 kWh/d. This parameter was calculated considereing the reference value of 21 MJ/m^3 of biogas as published in the Global Methane Initiative report.[43].

On the other hand, working with co-digestion (using more than one feedstock simultaneously), the CV is higher in co-digestion mode at the two model approaches reaching a maximum of 2,068 kWh/d·t (in SC8) and 2,075 kWh/d·t (in SC14). The electrical power potential (EPP) is calculated as the mass flow methane rate divided by 0.21 kg/kWh which is the methane consumption of a simple gas turbine[36]. EPP follows the same trend as CV due to the higher methane and biogas rates as highlighted in the literature[44] with a maximum of 1,037 kWh/d·t in co-digestion of all residues (SC8) and digestion with FW resulting in 1,922 kWh/d·t (SC10). Apart from EPP and CV, another advantage of co-digestion with two or more feedstocks is that it reduces the concentration of the inhibitors by increasing the ratio of the co-substrate.[45]

The last parameter appearing in Table 4, is the digestate-to-feedstock mass ratio obtained by dividing the residue resulted after AD (digestate mass flow) and the inlet flow of feedstock. The digestate is the by-product produced after the AD. The lowest ratios and consequently the highest AD efficiencies were: MSW digestion (0.5301), co-digestion with MSW and LCB (0.5314), co-digestion with MSW and FW (0.5363); and co-digestion with the three residues (0.5374). The digestate amounts are not negligible and in a circular bioeconomy concept, such byproduct (rich in nitrogen in the form of ammonium) should be used as an effective fertilizer for crop plants.[46] This concept is crucial especially in Iceland, where soil erosion issues and deforestation are some of the major environmental concerns of the country. Partial digestate concentrations can be also recirculated to the AD system for methane production, used as a substrate in bioethanol production, or even thermal converted through combustion, hydrothermal carbonization or pyrolysis, producing energy and improving the energy efficiency of the AD process.[47]

Two-stage in series AD model approach

The two digestion stages model approach was developed following the reactions of Rajendran model[33] in which there are two reaction sets: (i) hydrolysis, simulated in a stoichiometric reactor, which is the limiting factor in the AD process[48], based on the extent of reaction; (ii) acidogenic, acetogenic and methanogenic, simulated in a CSTR on a kinetic basis. Al-Rubaye[6] demonstrated how methane conversion efficiency ameliorates by adding a second digestion stage. Another reason for separating an AD plant using a two-stage AD configuration might be to control the pH range which optimum is different for hydrolysis, acidogenic, acetogenic or methanogenic reactions. Several two-stage AD models have been reported in the literature. [6,21,33,44] The two-stage AD model approach was performed at thermophilic conditions, so the results obtained could be compared with the ones obtained in the first model. Next, a summary of results of the two-stage AD model developed in this research is shown in Table 5.

Looking at the results from Table 5, biogas yields in the case of AD plants working in mono-digestion (one kind of feedstock) with high inlet waste streams of 300 t/d (SC9 to SC11), decrease when compared to the single-stage model. Nevertheless, the efficiency increased from 305.5 to 344.71 mL biogas/g VS working at 3 t/d of FW (SC12). Similarly, occurs with the methane yields, due to all reactions considered producing methane that was not included in the first model approach. In this case, AD plants operating with 3 t/d of FW (SC12) increased CH_4 yields from 68.62 up to 79.22 mL/g VS. Biogas yields of the proposed co-digestion scenarios are quite similar when the AD simulated plant operates with a mixture of all the bio residues collected by the SORPA facility. Looking at the results from Table 5, biogas yield in m^3/kg VS is in the range of 0.31 to 0.41 which is in accordance with the literature. Vasco-Correa et al.[2], reported biogas yields of animal manure (0.1-0.6 m^3/kg); MSW (0.3-0.6 (m^3/kg), FW (0.3-0.8 m^3/kg) among other feedstocks also used in this purpose. Barros et al.[49] also reported biogas yields of 0.1 m^3/kg for co-digestion of MSW and water sludge.

Regarding the methane yields observed in Table 5, all the simulated scenarios are in the range of 0.09-0.11 m^3 CH_4/kg VS. Such yields are also in accordance with the literature using as feedstocks organic fraction of MSW combined with sludge (0.0513 m^3/kg).[49]

Special attention should be taken with result obtained when LCB was used as feedstock. Looking at Table 5, regardless the inlet flow considered, the quantity of methane obtained was negligible compared with the scenarios that used this residue working with a single AD configuration. This effect is showed as well in Fig. 3, which represents the volume flow of the major biogas compounds (CH_4 and CO_2), for each scenario. This behavior can be explained with the Rajendran reaction schemes. Since there is no presence of protein and fatty acids in LCB. Proteins are degraded into H_3N and glycerol, respectively. Furthermore, NH_3 is a key component in amino acid degradation reactions, acetogenic, acidogenic and methanogenic stages as can be seen in Table 2. Fatty acids intervene in acetogenic reaction giving methane and hydrogen as the main products. As a results, none of this reactions take place and that is why methane yield is almost negligible.

Another significant difference between the configurations considered relies on the CO_2 generation (Fig 3). Due to the protein and fatty acids side reactions the concetration of CO_2 in the biogass, is always higher when using the two-stage AD model.

The total amount of the digestate varies between 1.92 t/d for 3 t/d AD plants and 200 t/d for 323 t/d AD plants. Nevertheless, looking at results from Table 5, the digestate-to-feedstock ratio is very similar. The digestate composition, is different when compared with the single-stage model approach because of all the amino acids reactions considered in the two-stage AD models. Looking at the digestate to feedstock ratio, in this case, more digestate is produced as it includes not only glycerol, ammonia, CO_2, CH_4, H_2S, cellulose, hemicellulose, protein or lignin but also amino acids, volatile fatty acids (VFAs), triolein, tripalmate, palmito olein, palmito linolein, protein and keratine that should be valorized into soil fertilizer or again recirculated to the system for optimizing the AD process.

Techno-economic and environmental aspects of the AD plants

Sizing and costing of the proposed scenarios were determined by the APEA Aspen tool. Besides, a summary of the total CO_2 equivalent emissions has also been estimated. AD plants working with 300 t/d to 323 t/d (co-digestion of MSW, FW and LCB) operating with hydraulic retention times of 15 days require digester volumes between 3800 and 4000 m^3 with respect to AD plants operating with inlet mass flows of 3 t/d (SC4 and SC12), require a digester volume of 38 m^3. Finally, AD plants operating with inlet mass flows of 20 t/d (SC5 and SC13) require vessels of 251 m^3. Such results are in agreement with the AP simulation performed by Harun et al.[50] who obtained reactor volume of 275 m^3 with inlet mass flows of 48 t/d.

The GHG in terms of equivalent carbon dioxide, CO_2eq, of all the simulated scenarios for both model approaches are plotted in Fig. 4. The two-stage AD model approach for all simulated scenarios is the best option from an environmental viewpoint.

In terms of total kg of CO_2eq per kg of feedstock, the single-stage model values are in the range of 0.080 to 0.111; the two-stage AD model approach scenarios are in the range of 0.00034-0.049 kg CO_2eq/kg waste. These results are better than the results of dairy cows AD plants in the range of 0.67 to 2.5 kg CO_2eq/kg waste.[51]

Total capital costs, operating costs, costs associated with utilities, equipment and installed costs determined by the APEA for the single-stage AD model approach are shown in Fig. 5. Capital costs of the single-stage model were between 3.57 million dollars (for the AD plant operating at 3 t/d of FW) and 4.49 million dollars (for the 323 t/d AD plant fed by the total average flow of the SORPA facility composed by MSW, FW and LCB). Due to the two separate digesters necessary for implementing the two-stage AD model approach, scenarios SC9 to SC16 have higher equipment cost, operating costs, utility costs and consequently higher capital costs. Therefore, scenarios of the single-stage model approach (SC1 to SC8) are optimum from an economic viewpoint.

Looking at results reported by Vasco-Correa et al.[2], capital cost in USD/t of a plant size between 1,000 and 10,000 t/year were 122,550 USD/t. The first three scenarios of this research with a plant size of 51,684 t of biogas/year (SC1 feed by MSW); 38,471 t of biogas/year (SC2 feed by FW); and 40,223 t of biogas/year (SC3 feed by LCB) are in the range studied by Vasco-Correa and resulted in capital costs of 14,961 USD/t (SC1); 14,741 USD/t (SC2) and 15,085 USD/t (SC3). Cavinato et al.[27] also reported capital cost evaluation of a medium-size biogas plant of 10,200 m3/d giving total cost of € 3,000,000. This value is in accordance with results of APEA because of SC1 to SC3 plants produce from 41,706 m^3/d and 96,558 m^3/d.

Models validation and sensitivity analysis

Validation of the models was done by calculating the theoretical volume of biogas per amount of inlet waste (in mL of biogas per g of dry waste). Such validation was done considering the conversion and stoichiometric factors followed in the methodology and densities of pure components at standard temperature and pressure (STP) as determined by Widiasa et al.[52] Before determining theoretical yields of this research, theoretical yield of cattle manure was calculated with the data of Widiasa et al.[52], giving results of 624 mL/g which is comparable to results of 618.9 mL/g obtained in the literature. Once the methodology was validated with results of cattle manure, simulations of this research based on MSW, FW and LCB were calculated. Thus, total theoretical biogas versus total biogas obtained in the simulations is shown in Fig. 6. Difference between theoretical and simulated biogas yields showed errors between 0.10 and 5.6 % in all the simulated scenarios. For this reason, we can conclude that simulation models correctly predict real behavior, yields and flow rates of a biogas plant.

Apart from the validation trough the theoretical biogas yield calculations, experimental data covering from small-scale laboratory research to large-scale industrial plants was used to corroborate the AP single-stage and two-stage AD models. Case studies presented by Rajendran et al.[33] and chosen to validate model approaches developed in this research were: (i) MSW in a 5 L volume reactor; (ii) an industrial AD plant operating in co-digestion of 75 % slaughterhouse waste, 15 % FW, and 10 % cow manure; (iii) pig manure in a 30 L volume reactor. Results of the model validation through experimental results are shown in Table 6. As can be seen in Table 6, both model fits well with the experimental study cases, regardless of the size of the AD plant (laboratory, pilot or industrial). So it can be concluded that all developed AP models are correct and can be used by SORPA landfill for their own purposes.

With the purpose of determining the effect of substrate concentration over the mass flow of methane presented in the biogas a sensitivity analysis was developed. Inlet feed of cellulose and hemicellulose varying from 0 to 300 t/d and inlet feed of protein and fats varying from 0 to 220 t/d was carried out. Results of the methane mass flow as a function of the inlet substrate mass flows in single-stage configuration is plotted in Fig. 7.

Linear relationship between cellulose, hemicellulose and protein load presented in the substrate and the CH_4 mass flow in biogas is shown in Fig. 7. Aparently there is not a possitive effect of fats substrate concentration over the production of CH_4. In fact, there is a slight donward linear trend with and slope of $-2\cdot10^{-4}$ (R^2=0.9962). Looking at results of the sensitivity analysis, the highest slope of Figure 7 and therefore the highest effect over the methane production, was to increase the hemicellulose substrate concentration (slope of 0.1518) followed by protein (slope of 0.1276) and cellulose (slope of 0.1087).

CONCLUSIONS

The biogas production from the waste stream of the Reykjavik capital area has been estimated for 16 realistic scenarios in order to identify the optimal production strategy, considering gas yields, CO_2 emissions and costs. All scenarios were simulated using the AspenPlusv10 software, using observed waste streams of MSW, FW and LCB between 2016 and 2019 and considering all relevant stoichiometric reactions occurring during anaerobic digestion. The highest biogas yield was reached using MSW as feedstock yielding 0.356 m^3 of biogas per kg of dry waste in SC1 and 0.359 m^3/kg in SC9. In regard to carbon emissions SC4, which is the smallest AD plant operating at 3 t/d of FW, giving 240 kg of CO_2eq per kg of waste. Comparing same AD plant sizes processing 300 t/d of waste, the best environmental friendly AD plant was the SC2 working with FW. SC2 revealed to produce 27.7 % lower emissions than SC1. This is mainly due to the fact that the higher fats and protein contents. In regard to operational costs the most cost effective is also the SC2 with capital costs of $14,741/t. Co-digestion scenarios for single-stage and two-stage AD models resulted the best values of methane EPP and biogas CV in comparison with scenarios working with one kind of feedstock. These results could be helpful to optimize biogas production. Furthermore, biogas operators might also switch between scenarios to optimize the production based on the current market situation. While these results are valid for the Reykjavik Capital area the approach presented could be applied to any municipality in the world.

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Table 1. Bio residues generation and composition in the Reykjavik area.

Feedstocks[1]	MSW	LCB	FW
2016 (t/y)	104,504	7,130	1,067
2017 (t/y)	118,817	7,542	1,063
2018 (t/y)	120,027	8,633	1,614
2019 (t/y)	107,340	8,633	1,169
Q_{feed} (t/day)	300	20.0	3.00
Carbohydrates (t/day)	185	-	1.13
Protein (t/day)	48.0	-	0.52
Lipids (t/day)	30.0	-	0.90
Cellulose (t/day)	-	7.42	-
Hemicellulose (t/day)	-	5.98	-
Lignin (t/day)	-	3.52	-
Water (t/day)	37.5	3.08	0.46

[1] All data was provided by the waste company SORPA in Reykjavik, Iceland

Table 2. Reactions scheme for Model 2 using the two-stages model approach.

No	Component	Reaction	Extent of reaction
1	Cellulose	$(C_6H_{12}O_6)_n + H_2O \rightarrow n\ C_6H_{12}O_6$	0.4 ± 0.1
2	Hemicellulose	$C_5H_8O_4 + H_2O \rightarrow 2.5\ C_2H_4O_2$	0.5 ± 0.2
3	Hemicellulose	$C_5H_8O_4 + H_2O \rightarrow C_5H_{10}O_5$	0.6 ± 0.0
4	Xylose	$C_5H_{10}O_5 \rightarrow C_5H_4O_2 + 3H_2O$	0.6 ± 0.0
5	Cellulose	$C_6H_{12}O_6 + H_2O \rightarrow 2C_2H_6O + 2CO_2$	0.4 ± 0.1
6	Ethanol	$2C_2H_6O + CO_2 \rightarrow 2C_2H_4O_2 + CH_4$	0.6 ± 0.1
7	Soluble protein	$C_{13}H_{25}O_7N_3S + 6H_2O \rightarrow 6.5\ CO_2 + 6.5CH_4 + 3H_3N + H_2S$	0.5 ± 0.2
8	Insoluble protein (IP)	$IP+0.3337H_2O \rightarrow 0.045C_6H_{14}N_4O_2+0.048C_4H_7NO_4+0.047C_4H_9NO_3+0.172C_3H_7NO_3+0.074C_5H_9NO_4+0.111C_5H_9NO_2+0.25C_2H_5NO_2+0.047C_3H_7NO_2+0.067C_3H_6NO_2S+0.074C_5H_{11}NO_2+0.07C_6H_{13}NO_2+0.046C_6H_{13}NO_2+0.036C_9H_{11}NO_2$	0.6 ± 0.1
9	Triolein	$C_{57}H_{104}O_6+3H_2O \rightarrow C_3H_8O_3+3C_{18}H_{34}O_2$	0.5 ± 0.2
10	Tripalmate	$C_{51}H_{98}O_6+8.436H_2O \rightarrow 4C_3H_8O_3+2.43C_{16}H_{34}O_2$	0.5 ± 0.3
11	Palmito-olein	$C_{37}H_{70}O_5+4.1H_2O \rightarrow 2.1C_3H_8O_3+0.9C_{16}H_{34}O+0.9C_{18}H_{34}O_2$	0.6 ± 0.2
12	Palmito-linolein	$C_{37}H_{68}O_5+4.3H_2O \rightarrow 2.2C_3H_8O_3+0.9C_{16}H_{34}O+0.9C_{18}H_{32}O_2$	0.6 ± 0.2

No	Component	Reaction	Kinetic constant K
		Amino acid degradation reactions	
1	Glycine	$C_2H_5NO_2+H_2 \rightarrow C_2H_4O_2+H_3N$	$1.28 \cdot 10^{-2}$
2	Threonine	$C_4H_9NO_3+H_2 \rightarrow C_2H_4O_2+0.5C_4H_8O_2+H_3N$	$1.28 \cdot 10^{-2}$
3	Histidine	$C_6H_8N_3O_2+4H_2O+0.5H_2 \rightarrow CH_3NO+C_2H_4O_2+0.5C_4H_8O_2+2H_3N$	$1.28 \cdot 10^{-2}$
4	Arginine	$C_6H_{14}N_4O+3H_2O+H_2 \rightarrow 0.5C_2H_4O_2+0.5C_3H_6O_2+0.5C_5H_{10}O_2+4H_3N+CO_2$	$1.28 \cdot 10^{-2}$
5	Proline	$C_5H_9NO_2+H_2O+H_2 \rightarrow 0.5C_2H_4O+0.5C_3H_6O_2+0.5C_5H_{10}O_2+H_3N$	$1.28 \cdot 10^{-2}$
6	Methionine	$C_5H_{11}NO_2S+2H_2O \rightarrow C_3H_6O_2+CO_2+H_3N+H_2+CH_4S$	$1.28 \cdot 10^{-2}$
7	Serine	$C_3H_7NO_3+H_2O \rightarrow C_2H_4O_2+H_3N+CO_2+H_2$	$1.28 \cdot 10^{-2}$
8	Threonine	$C_4H_9NO_3+H_2O \rightarrow C_3H_6O_2+H_3N+H_2+CO_2$	$1.28 \cdot 10^{-2}$
9	Aspartic acid	$C_4H_7NO_4+2H_2O \rightarrow C_2H_4O_2+H_3N+2CO_2+2H_2$	$1.28 \cdot 10^{-2}$
10	Glutamic acid	$C_5H_9NO_4+H_2O \rightarrow C_2H_4O_2+0.5C_4H_8O_2+H_3N+CO_2$	$1.28 \cdot 10^{-2}$
11	Glutamic acid	$C_5H_9NO_4+2H_2O \rightarrow 2C_2H_4O_2+C_4H_8O_2+H_3N+CO_2$	$1.28 \cdot 10^{-2}$
12	Histidine	$C_6H_8N_3O_2+5H_2O \rightarrow CH_3NO+2C_2H_4O_2+2H_3N+CO_2+0.5H_2$	$1.28 \cdot 10^{-2}$
13	Arginine	$C_6H_{14}N_4O_2+6H_2O \rightarrow 2C_2H_4O_2+4H_3N+2CO_2+3H_2$	$1.28 \cdot 10^{-2}$
14	Lysine	$C_6H_{14}N_2O_2+2H_2O \rightarrow C_2H_4O_2+C_4H_8O_2+2H_3N$	$1.28 \cdot 10^{-2}$
15	Leucine	$C_6H_{13}NO_2+2H_2O \rightarrow C_5H_{10}O_2+H_3N+CO_2+2H_2$	$1.28 \cdot 10^{-2}$
16	Isoleucine	$C_6H_{13}NO_2+2H_2O \rightarrow C_5H_{10}O_2+H_3N+CO_2+2H_2$	$1.28 \cdot 10^{-2}$
17	Valine	$C_5H_{11}NO_2+2H_2O \rightarrow C_4H_8O_2+H_3N+CO_2+2H_2$	$1.28 \cdot 10^{-2}$

Table 2. (Cont.)

No	Component	Reaction	Kinetic
18	Phenyalanine	$C_9H_{11}NO_2+2H_2O \rightarrow C_6H_6+C_2H_4O_2+H_3N+CO_2+H_2$	$1.28\cdot10^{-2}$
19	Tyrosine	$C_9H_{11}NO_3+2H_2O \rightarrow C_6H_6O+C_2H_4O_2+H_3N+CO_2+H_2$	$1.28\cdot10^{-2}$
20	Typtophan	$C_{11}H_{12}N_2O_2+2H_2O \rightarrow C_8H_7N+C_2H_4O_2+H_3N+CO_2+H_2$	$1.28\cdot10^{-2}$
21	Glycine	$C_2H_5NO_2+0.5H_2O \rightarrow 0.75C_2H_4O_2+H_3N+0.5CO_2$	$1.28\cdot10^{-2}$
22	Alanine	$C_3H_7NO_2+2H_2O \rightarrow C_2H_4O_2+H_3N+CO_2+2H_2$	$1.28\cdot10^{-2}$
23	Cysteine	$C_3H_6NO_2S+2H_2O \rightarrow C_2H_4O_2+H_3N+CO_2+0.5H_2+H_2S$	$1.28\cdot10^{-2}$
		Acidogenic reactions	
24	Dextrose	$C_6H_{12}O_6+0.1115H_3N \rightarrow 0.1115C_5H_7NO_2+0.74C_2H_4O_2+0.5C_3H_6O_2+0.4409C_4H_8O_2+0.6909CO_2+1.0254H_2O$	$9.54\cdot10^{-3}$
25	Glycerol	$C_3H_8O_3+0.4071H_3N+0.0291CO_2+0.0005H_2 \rightarrow 0.04071C_5H_7NO_2+0.94185C_3H_6O_2+1.09308H_2O$	$1.01\cdot10^{-2}$
		Acetogenic reactions	
26	Oleic acid	$C_{18}H_{34}O_2+15.2396H_2O+0.2501CO_2+0.1701H_3N \rightarrow 0.1701C_5H_7NO_2+8.6998C_2H_4O_2+14.4978H_2$	$3.64\cdot10^{-12}$
27	Propionic acid	$C_3H_6O_2+0.06198H_3N+0.314336H_2O \rightarrow 0.06198C_5H_7NO_2+0.9345C_2H_4O_2+0.660412CH_4+0.160688CO_2+0.00055H_2$	$1.95\cdot10^{-7}$
28	Isobutyric acid	$C_4H_8O_2+0.0653H_3N+0.8038H_2O+0.0006H_2+0.5543CO_2 \rightarrow 0.0653C_5H_7NO_2+1.8909C_2H_4O_2+0.446CH_4$	$5.88\cdot10^{-6}$
29	Isovaleric acid	$C_5H_{10}O_2+0.0653H_3N+0.5543CO_2+0.8044H_2O \rightarrow 0.0653C_5H_7NO_2+0.8912C_2H_4O_2+C_3H_6O_2+0.4454CH_4+0.0006H_2$	$3.01\cdot10^{-8}$
30	Linoleic acid	$C_{18}H_{32}O_2+15.356H_2O+0.482CO_2+0.1701H_3N \rightarrow 0.1701 C_5H_7NO_2+9.02C_2H_4O_2+10.0723H_2$	$3.64\cdot10^{-12}$
31	Palmitic acid	$C_{16}H_{34}O+15.235H_2O+0.482CO_2+0.1701H_3N \rightarrow 0.1701C_5H_7NO_2+8.4404C_2H_4O_2+14.974H_2$	$3.64\cdot10^{-12}$
		Methanogenic reactions	
32	Acetic acid	$C_2H_4O_2+0.022H_3N \rightarrow 0.022C_5H_7NO_2+0.945CH_4+0.066H_2O+0.945CO_2$	$2.39\cdot10^{-3}$
33	Hydrogen	$14.4976H_2+3.8334CO_2+0.0836H_3N \rightarrow 0.0836C_5H_7NO_2+3.4154CH_4+7.4996H_2O$	$2.39\cdot10^{-3}$

Table 3. Scenarios of biogas production tested in the AP developed models

Scenario (SC)	**Model**	**Feedstock**	**Inlet Flow waste (t/d)**
SC1	AP single-stage	MSW	300
SC2	AP single-stage	FW	300
SC3	AP single-stage	LCB	300
SC4	AP single-stage	FW	3.00
SC5	AP single-stage	LCB	20.0
SC6	AP single-stage	All residues	323
SC7	AP single-stage	MSW & FW	303
SC8	AP single-stage	MSW & LCB	320
SC9	AP two-stage	MSW	300
SC10	AP two-stage	FW	300
SC11	AP two-stage	LCB	300
SC12	AP two-stage	FW	3.00
SC13	AP two-stage	LCB	20.0
SC14	AP two-stage	All residues	323
SC15	AP two-stage	MSW & FW	303
SC16	AP two-stage	MSW & LCB	320

Table 4. Model results of the single-stage stoichiometric model approach.

Scenario (SC)	SC1	SC2	SC3	SC4	SC5	SC6	SC7	SC8
Feedstock	MSW	FW	LCB	FW	LCB	All residues	MSW & FW	MSW & LCB
Inlet flow (t/d)	300.0	300.0	300.0	3.000	20.00	323.0	303.0	320.0
Biogas yield (mL/g VS)	406.4	305.5	380.5	305.5	380.5	404.2	405.2	405.3
Methane yield (mL/g VS)	89.19	68.62	106.0	68.62	106.0	88.82	89.01	88.97
Digestate to feedstock ratio (g:g)	0.5301	0.6509	0.6349	0.6509	0.6349	0.5374	0.5363	0.5314
Calorific value of biogas (kWh/d)	622,326	453,288	563,288	4,533	37,550	664,752	660,383	626,604
Electrical potential (kWh/d)	311,866	240,926	186,362	2,409	12,424	327,193	324,836	314,156

Table 5. Model results of the two-stage model approach.

Scenario (SC)	**SC9**	**SC10**	**SC11**	**SC12**	**SC13**	**SC14**	**SC15**	**SC16**
Feedstock	MSW	FW	LCB	FW	LCB	All residues	MSW & FW	MSW & LCB
Inlet flow (t/d)	300.0	300.0	300.0	3.000	20.00	323.0	303.0	320.0
Biogas yield (mL/g VS)	358.8	333.4	64.78	344.71	65.39	339.5	339.5	358.7
Methane yield (mL/g VS)	71.01	79.18	$8.2 \cdot 10^{-9}$	79.22	$1.6 \cdot 10^{-5}$	66.81	66.70	71.07
Digestate to feedstock ratio (g:g)	0.5965	0.6576	0.9156	0.6400	0.9151	0.6178	0.6174	0.2463
Calorific value of biogas (kWh/d)	549,398	494,719	95,903	5,117	6,454	558,345	553,393	554,435
Electrical potential (kWh/d)	58,316	63,018	$6.5 \cdot 10^{-6}$	631	$8.4 \cdot 10^{-4}$	58,936	58,306	58,924

Table 6. Validation of AP single-stage and AP two-stage models with experimental data.

Loading rate	Feedstock	Composition	Reactor volume	Biogas yield	AP single-stage	AP two-stage
150 m^3/d	co-dig of FW, Cow manure and slaughterhouse	23.5 % carbohydrates 12.18 % proteins 60 % fats	3700 m^3	10959 m^3/d	11110 m^3/d	11032 m^3/d
0,2304 kg/d	pig manure	44.6 % carbohydrates 23 % proteins 4.9 % fats	0.03 m^3	0,269 m^3/kg	0.331 m^3/kg	0.289 m^3/kg
3 $kg/m^3\cdot d$	MSW	61.5 % carbohydrates 16 % proteins 10 % fats	$5\cdot10^{-3}$ m^3	3 $kg/m^3\cdot d$	4.15 $kg/m^3\cdot d$	3.94 $kg/m^3\cdot d$

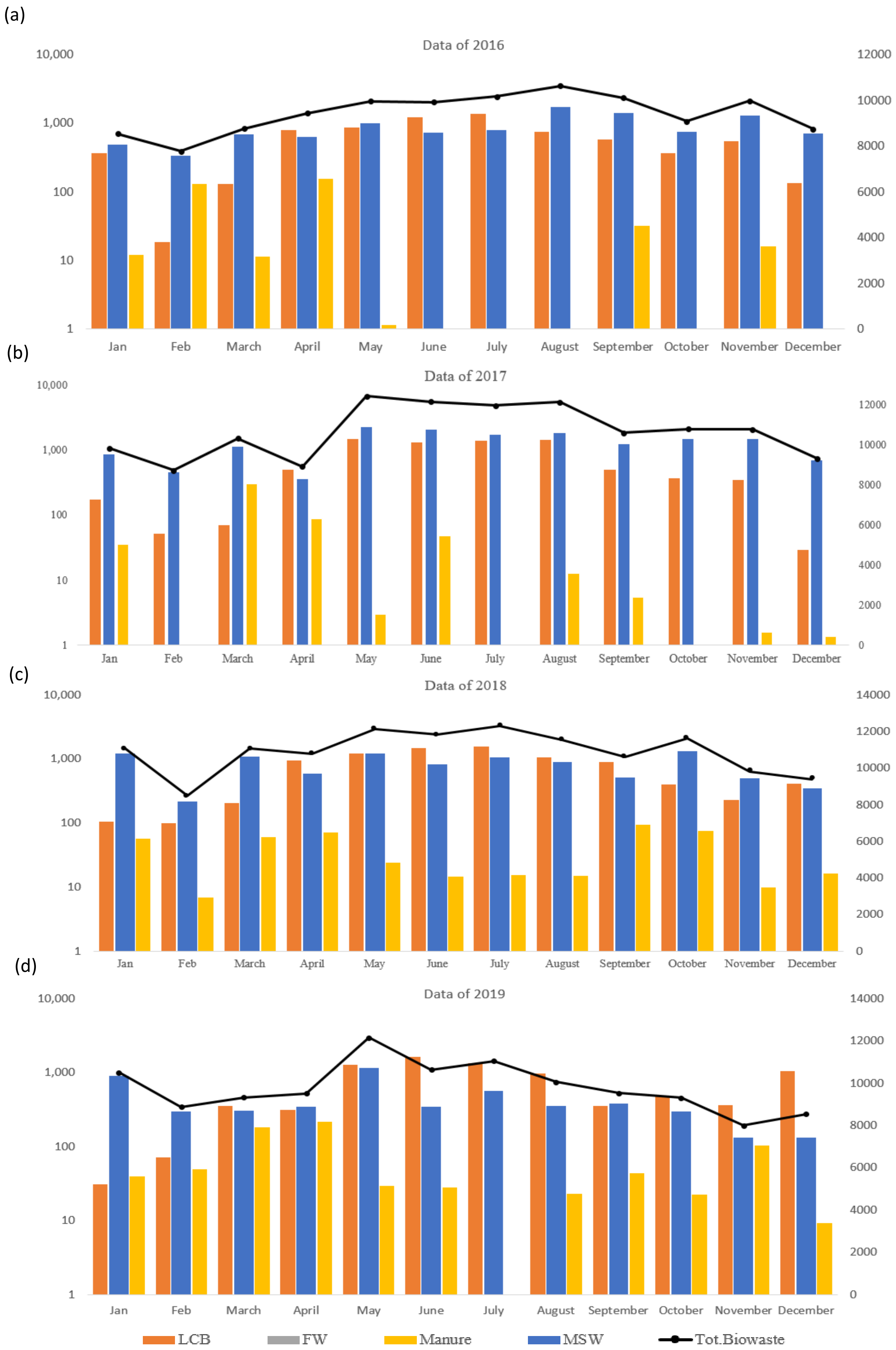

Figure 1. Seasonal evolution of the bio residues generated in: (a) 2016; (b) 2017; (c) 2018; and (d) 2019.

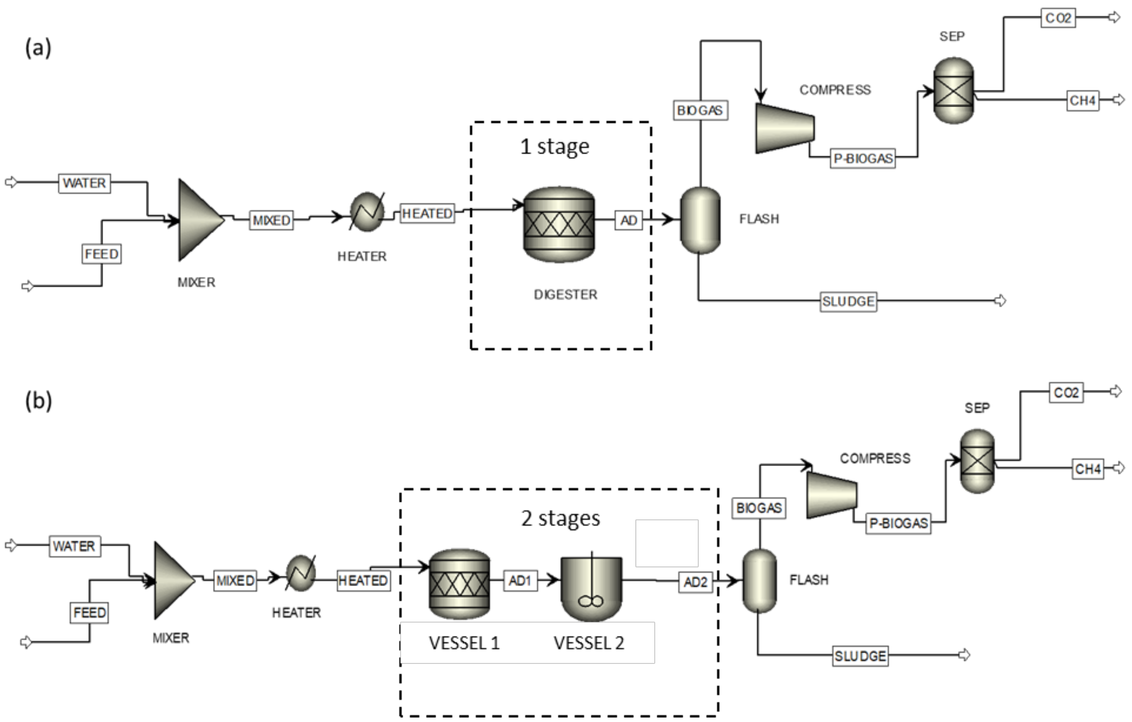

Figure 2. Flowsheet of the AP model approaches: (a) single-stage AD model; (b) two-stage AD model.

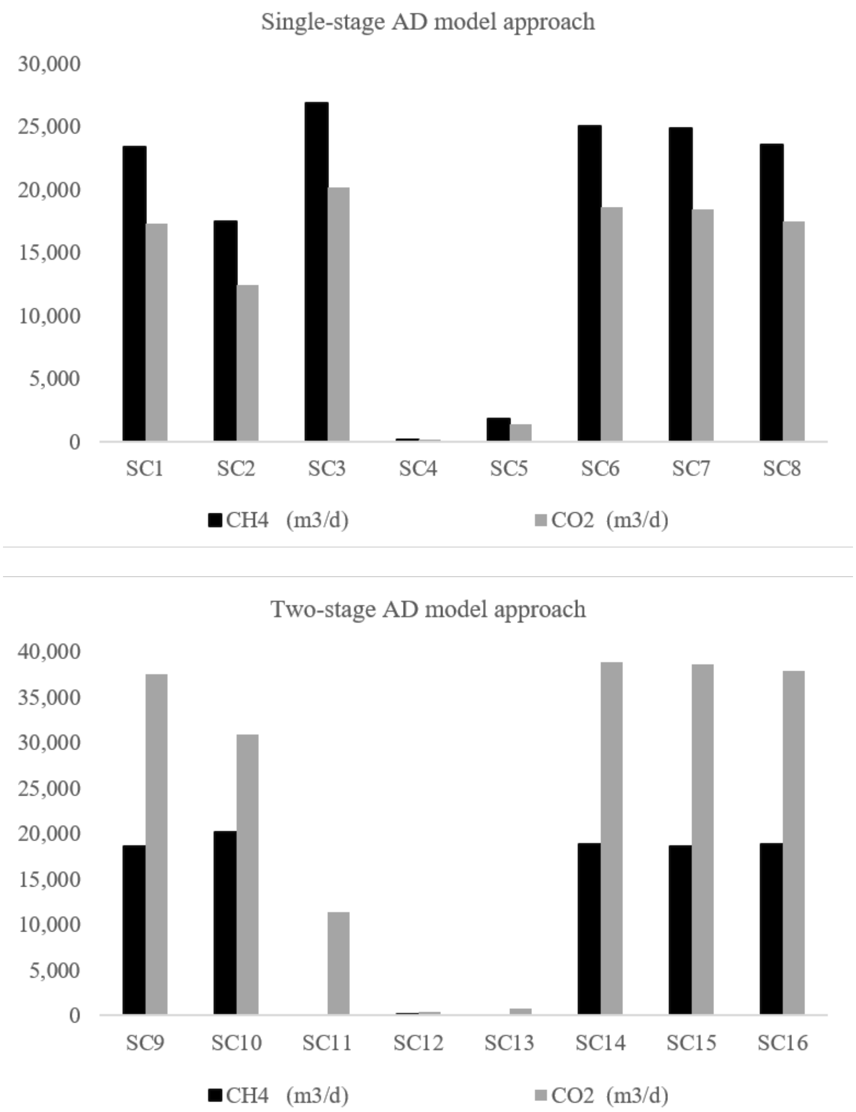

Figure 3. Graph bars of daily rate of CH_4 and CO_2 in single-stage and two-stage AP model approaches.

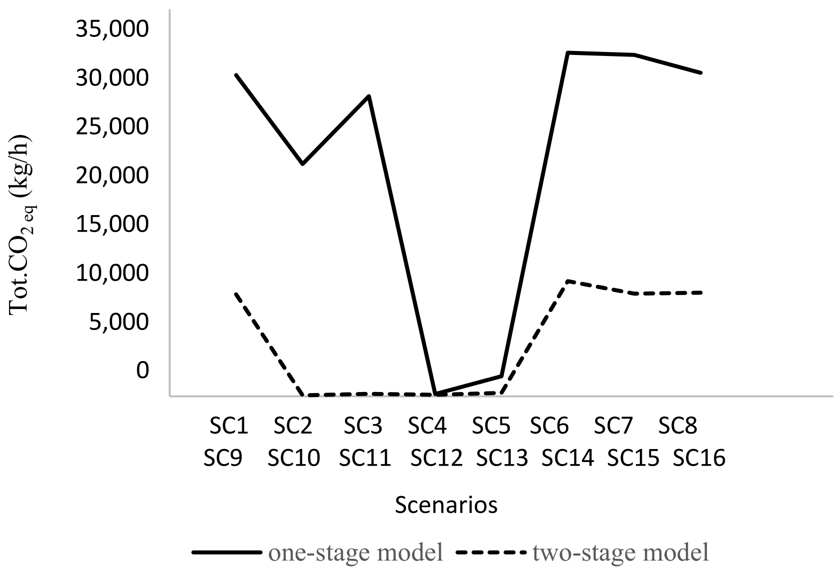

Figure 4. Total CO_2 equivalent of the AD simulated scenarios for the two model approaches.

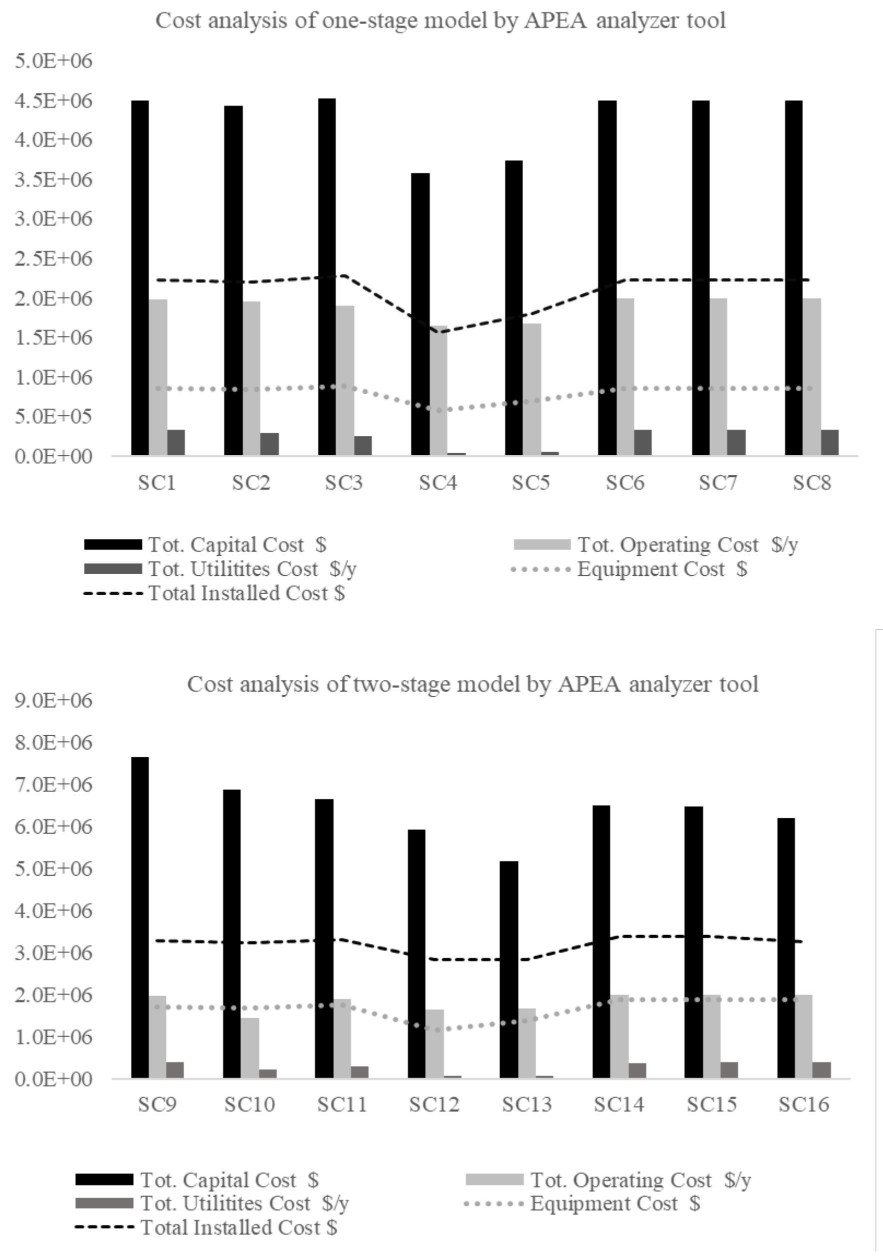

Figure 5. Cost analysis of the scenarios developed in Aspen Plus: (a) single-stage model approach; (b) two-stage model approach.

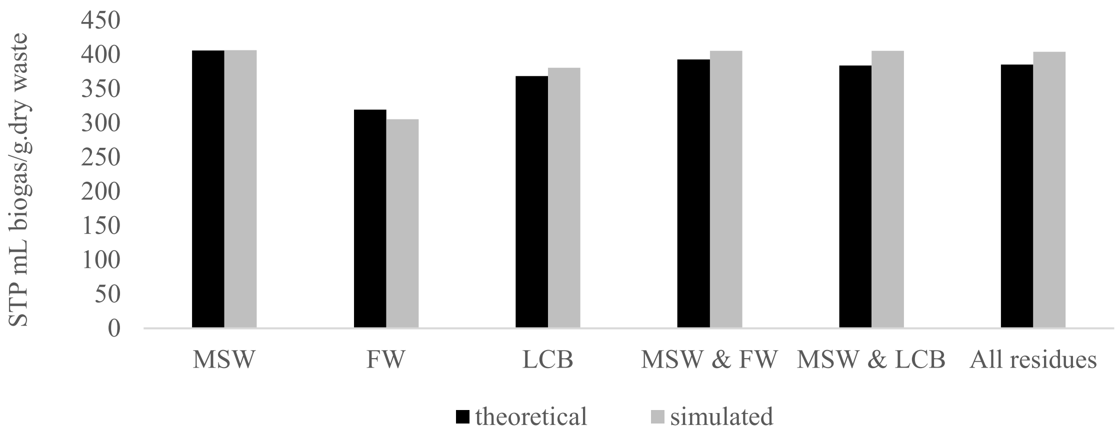

Figure 6. Theoretical and simulated biogas yields.

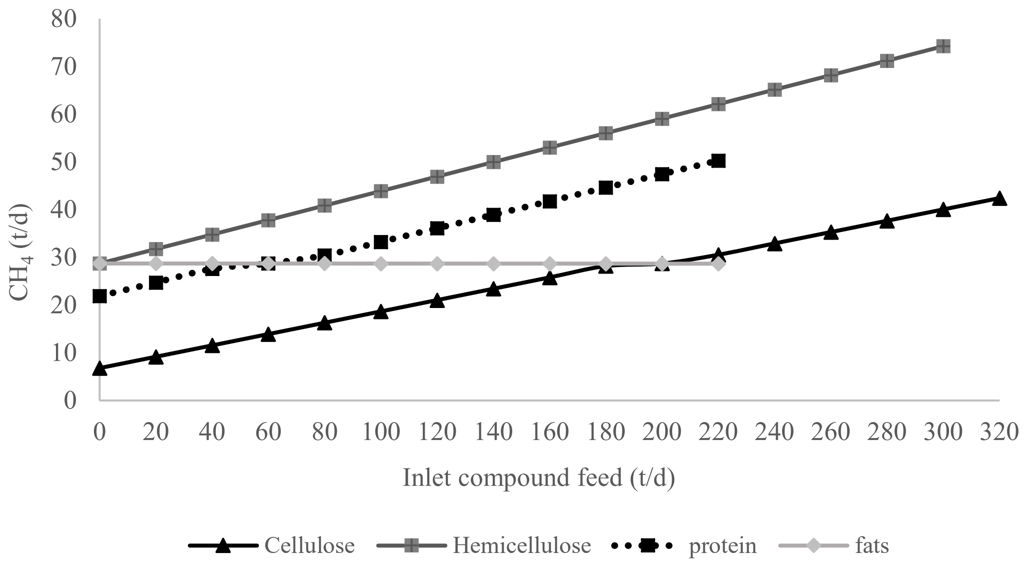

Figure 7. Sensitivity analysis of the methane mass flow at different substrate concentrations.