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# The Effect of Hydrogen Peroxide on Biogas and Methane Produced from Batch Mesophilic Anaerobic Digestion of Spent Coffee Grounds

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**Abstract:** This paper aims to explore both experimental and modeling anaerobic digestion (AD) processes as innovative methods for managing the substantial quantities of spent coffee grounds (SCG) generated in Algeria, transforming them into valuable renewable energy sources (biogas/methane). AD of SCG, while promising, is hindered by its complex lignocellulosic structure, which poses a significant challenge. This study investigates the efficacy of hydrogen peroxide ( $H_2O_2$ ) pretreatment in addressing this issue, with a particular focus on enhancing biogas and methane production. The AD of SCG was conducted over a 46-day period, and the impact of  $H_2O_2$  pretreatment was evaluated using laboratory-scale batch anaerobic reactors. Four different concentrations of  $H_2O_2$  (0.5, 1, 2, and 4%  $H_2O_2$  *w/w*) were studied in mesophilic conditions ( $37 \pm 2$ ) for 24 h at room temperature, providing basic data on biogas and methane production. The results showed a significant increase in soluble oxygen demand (SCOD) and total sugar solubilization in the range of 555.96–713.02% and 748.48–817.75%, respectively. The optimal pretreatment was found to be 4%  $H_2O_2$  *w/w* resulting in 16.28% and 16.93% improvements in biogas and methane yield over the untreated SCG. Further, while previous research has established oxidative pretreatment efficacy, this study uniquely combines the empirical analysis of  $H_2O_2$  pretreatment with a detailed kinetic modeling approach using the modified Gompertz (MG) and logistic function (LF) models to estimate kinetic parameters and determine the accuracy of fit. The MG model showed the most accurate prediction, thus making the present investigation a contribution to understanding the performance of the AD system under oxidative pretreatment and designing and scaling up new systems with predictability. These findings highlight the potential of  $H_2O_2$ -pretreated SCG as a more efficient and readily available resource for sustainable waste management and renewable energy production.



Academic Editor: Alessia Tropea

Received: 9 December 2024

Revised: 23 January 2025

Accepted: 25 January 2025

Published: 29 January 2025

**Citation:** Sayoud, S.; Derbal, K.; Panico, A.; Pontoni, L.; Fabbricino, M.; Pirozzi, F.; Benalia, A. The Effect of Hydrogen Peroxide on Biogas and Methane Produced from Batch Mesophilic Anaerobic Digestion of Spent Coffee Grounds. *Fermentation* **2025**, *11*, 60. <https://doi.org/10.3390/fermentation11020060>

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**Keywords:** biogas; methane; anaerobic digestion; batch mesophilic;  $H_2O_2$

## 1. Introduction

The world's energy needs have been heavily dependent on fossil fuels. Depleting fossil fuel reserves and global warming have urged man to look for feasible, eco-friendly alternatives for sustainable energy [1]. In recent years, renewable energy has come to the forefront, and biomass is the world's fourth largest energy source [2–4] and is, without a doubt, the most flexible [5]. The anaerobic digestion (AD) of biomass residues is considered one of the sustainable options for producing green energy to meet global demand and ensure an adequate future supply of clean energy and fuel [6]. Therefore, it has been widely used to manage various organic wastes, such as food waste, animal manure, and sewage sludge [6–9].

Nowadays, coffee is, after water, the second most popular beverage worldwide and the second largest commodity in the stock exchange after oil [7]. Algeria, ranked by the International Coffee Organization (ICO) as the second largest coffee consumer in Africa, consumed 1.8 million 60 kg bags of coffee in the 2022/23 coffee year (ICO, December 2023). This substantial coffee consumption generates a considerable amount of spent coffee grounds (SCG), the byproduct remaining after coffee brewing. Based on a reported SCG generation rate of 650 kg per ton of green coffee [8], and assuming the imported coffee is primarily green coffee, this consumption level translates into an estimated annual SCG production exceeding 0.7 million tons. This substantial volume of organic waste represents both a significant disposal challenge and a promising opportunity for bioenergy production. The management of municipal solid waste is one of the most significant challenges for the effective implementation of the circular economy. An innovative approach currently being proposed involves the use of anaerobic reactors for the treatment of waste streams [9]. The collection of SCG for industrial AD facilities would need to involve different sources, mainly restaurants, coffee shops, cafeterias, and households, with organized collection strategies that could be performed with collaboration between local authorities, private waste management companies, and coffee shop owners. These logistical challenges are critical to consider in the planning and implementation of SCG valorization projects. Thus, an alternative way of treating, or even better, valorizing SCG was sought [10]. At present, there are a variety of options for the utilization of SCG in the field of agriculture [8] and numerous possibilities for converting SCG to biofuels [2]. It can be converted to produce various types of biofuels such as fuel pellets [2], biodiesel [11,12], bioethanol [12,13], biogas [14], and biomethane [5,15].

Among all the biofuels, biogas is paid increasing attention because its production process and conditions are simpler than the production of other biofuels, which makes biogas production more practical [16]. The production of biogas from SCG constitutes an alternative "green" technological scheme aiming to produce renewable energy while biologically treating SCG [10]. Its high organic content means that it is an attractive feedstock for AD, and many studies have investigated its biomethanation potential [17]. Biomethane presents an environmentally friendly replacement for natural gas, finding applications in transportation, heating, and electricity generation. There is a rising interest in developing methods for cost-effective and sustainable production [18]. SCG is rich in cellulose and hemicellulose polysaccharides and can be considered lignocellulosic residues [19]. Thus, pretreatment is an essential step to degrade the recalcitrant lignocellulosic fibers and facilitate the subsequent step of enzymatic hydrolysis [13].

Among all the pretreatments reported in the literature, chemical treatment is the most common and intensively studied method for lignocellulosic biomass in the AD process [16]. Hydrogen peroxide has been chosen to enhance biogas yield, which is a strong oxidant that has the significant advantage of leaving no residues in the biomass because it degrades into oxygen and water and hardly forms secondary products [6].

This study addresses the aforementioned challenges by evaluating the impact of different  $\text{H}_2\text{O}_2$  concentrations on SCG anaerobic digestibility. We analyze the effects of  $\text{H}_2\text{O}_2$  pretreatment using both experimental and numerical methods. The primary goals are to assess the impact of hydrogen peroxide concentration (0.5%, 1%, 2%, and 4%) on (1) the solubilization of organic material (SCOD and Total Sugars) and (2) cumulative biogas and methane yields and to (3) model the kinetics of the methane production process to accurately predict the process performance for enhanced biogas production. By using this approach, we intend to determine the optimal conditions for  $\text{H}_2\text{O}_2$  pretreatment to enhance the efficiency of AD for SCG, providing valuable insight for sustainable waste management and renewable energy production.

## 2. Materials and Methods

### 2.1. Sample Collection and Characteristics

Activated sludge (AS) used as inoculum for the batch test was collected from the wastewater treatment plant (WWTP) of Oued El-Athmania, located in Mila (Algeria). SCG was collected from a cafeteria in the student club building of SALAH BOUBNIDR University, Constantine, Algeria. After collection, the samples were oven-dried at 60 °C for two or three days to a moisture content of less than 10% and stored in sealed plastic bags at room temperature until use [20]. This is a common practice in anaerobic digestion studies to ensure consistency in substrate composition and prevent microbial activity during storage.

The properties of the SCG and the AS are shown in Table 1.

**Table 1.** Selected composition characteristics of the SCGs and inoculum used in the experiment.

Parameter	Unit	SCG	Inoculum
Total solids (TS)	g/L	899.856 ± 7.41	37.536 ± 1.365
Total volatile solids (TVS)	g/L	889.833 ± 7.562	18.5363 ± 0.353
TVS/TS	%	98.886	49.383
pH	/	5.68 ± 0.025	6.7 ± 0.175
Total chemical oxygen demand (COD)	go <sub>2</sub> /L	44.792 ± 4.886	14.461 ± 0.121
Soluble chemical oxygen demand (SCOD)	go <sub>2</sub> /L	4.322 ± 0.141	0.373 ± 0.005
Total nitrogen Kjeldahl (TKN)	g/kg	2.216 ± 0.126	2.282 ± 0.042
ammonium nitrogen (N-NH <sub>4</sub> <sup>+</sup> )	mg/L	1.002 ± 0.026	0.043 ± 0.001
Protein	g/kg	13.850 ± 0.602	14.263 ± 0.262
Total alkalinity	mgCaCO <sub>3</sub> /L	327.61 ± 8.452	1178.31 ± 81.691

### 2.2. Oxidative Pretreatment

Tests were carried out in 500 mL digestion flasks, in which samples of 200 g of SCG were soaked in 400 mL of hydrogen peroxide ( $\text{H}_2\text{O}_2$ ) solution at room temperature for 24 h. The corresponding  $\text{H}_2\text{O}_2$  loadings over the substrate solids were 0.5, 1, 2, and 4% *w/w*, respectively. SCG soaked in tap water and stored as above, but without chemical pretreatment, was used as the control. The impact of hydrogen peroxide on the morphological structure of lignocellulosic substrates, mediated by its delignifying action, has been previously demonstrated [21], and the formation of reactive free radicals, such as hydroxyl ( $\text{HO}\bullet$ ) and hydroperoxyl ( $\text{HO}_2\bullet$ ), promotes organic matter decomposition [22].

### 2.3. Biochemical Methane Production (BMP) Tests

The tests were carried out in 120 mL serum bottles. Each bottle was fed an appropriate amount of a substrate and inoculum, the ratio between the volatile solids of the substrate to be degraded and volatile solids of the inoculum biomass (S/I) was kept constant at 2:1 for all tests [23], and 0.75 g of  $\text{NaHCO}_3$ /g TS was added to ensure suitable alkalinity and maintain a pH of around 7. Blank tests using the inoculum alone were also prepared to

measure the quantity of methane produced only by the biomass. All bottles were flushed with pure argon for 3–4 min to maintain anaerobic conditions. The prepared bottles were plugged with butyl rubber stoppers and aluminum seals, and they were incubated at  $37 \pm 2$  °C until the production of biogas became very meager. All tests were performed in triplicate. The biogas flow is measured by means of the water replacement method. The cumulative biogas production was calculated by subtracting the control.

#### 2.4. Analytical Methods

The total solid (TS), volatile solid (VS), pH, soluble chemical oxygen demand (SCOD), total chemical oxygen demand in SCG (TCOD), total nitrogen Kjeldahl (TKN), ammonia ( $\text{NH}_4^+$ ), and alkalinity were determined according to APHA (1998). The protein content was estimated by multiplying the total Kjeldahl nitrogen by a factor of 6.25, and the total sugars were determined by the phenol-sulfuric acid method. The methane proportions (%) in biogas were determined using the KOH saturated-solution method.

#### 2.5. Kinetic Study

Most of the equations describing a sigmoidal growth curve contain mathematical parameters ( $a, b, c, \dots$ ) rather than parameters with a biological meaning ( $A, \mu_m$ , and  $\lambda$ ). Therefore, all the growth models were rewritten to substitute the mathematical parameters with  $A, \mu_m$ , and  $\lambda$ . This was achieved by deriving an expression of the biological parameters as a function of the parameters of the basic function and then substituting them in the formula [24]. The Gompertz model is one of the most frequently used sigmoid models fitted to growth data and other data, perhaps only second to the logistic model. The re-parameterization proposed by Zwietering and colleagues is often called a “modified Gompertz” and is typically applied to bacterial growth data, especially in food [25].

According to previous studies in the literature, the modified Gompertz model [26,27] and the logistic function [27,28] are proposed to calculate the kinetic parameters of the AD process. The equations of the two models are as follows:

$$Y = A * \exp \left[ -\exp \left( \frac{\mu_m * e}{A} \right) * (\lambda - t) + 1 \right] \quad (1)$$

$$Y = \frac{A}{\left[ 1 + \exp \left( \frac{4 * \mu_m}{A} \right) * (\lambda - t) + 2 \right]} \quad (2)$$

where  $Y$  is the cumulative methane production (mL/g VS),  $\mu_m$  is the maximum methane production (mL/g VS/day),  $t$  is the time (day),  $A$  is the methane production potential (mL/g VS),  $\lambda$  is the lag phase (day), and  $e$  is the mathematical constant equivalent to 2.718.

The curve fitting and estimation of kinetic parameters of the modified Gompertz model and the logistic model were performed using Origin Pro 8 software supplied by Origin Lab. The experimental outputs obtained from all reactors were checked for the fitness of the models, and the effectiveness of the models' fit was assessed by statistical indicators, which were determined and compared: the correlation coefficient ( $R^2$ ) and the root mean square error (RMSE).

### 3. Results

#### 3.1. Effect of Hydrogen Peroxide Pretreatment on the Chemical Composition of SCG

The chemical composition of SCG is directly linked to the initial coffee beans. Their composition varies with the bean variety, cultivation conditions, processing methodology [10], brewing conditions applied, or secondary raw materials involved in the process of brewing [13]. The characteristics of the pretreated and not pretreated SCG used in this study, expressed in terms of major parameters, are presented in Table 1.

Regarding SCG, the TVS/TS ratio in this work reached 98.88%, which is approximately the same as that reported in the literature. Kim, J., et al. found (TVS/TS = 98%) [29], whereas Li et al. reported (TVS/TS = 98.4%) [26]. Therefore, SCG showed the highest VS content in dry basic weight, which was preferred for AD.  $H_2O_2$  pretreatment caused the TS and TVS content to decrease by 4.54–25.36% and 1.76–24.79%, respectively, compared to the control, while the lowest reduction was observed with 2%  $H_2O_2$  *w/w*.

Total alkalinity (TA) indicates the buffering capacity to neutralize acids, which could protect against the low pH of the AD system [16]. Moreover, adequate alkalinity is very necessary to maintain the pH of the reactor [30]. In this work, alkalinity was observed in the range of 257.02 to 354.76 mgCaCO<sub>3</sub>/L. The lowest value was noted with 2%  $H_2O_2$  *w/w*.

Pretreatment with  $H_2O_2$  decreased the total nitrogen Kjeldahl (TKN) concentrations from 2.22 to 1.91 g/L and released ammonium nitrogen (N-NH<sub>4</sub><sup>+</sup>) from 1.00 to 1.31 g/L. Therefore, it led to the degradation of protein ranging between 6.14 and 13.63%, while the highest amount was obtained with 2%  $H_2O_2$  *w/w*.

The directly observable impact of alkaline  $H_2O_2$  treatment was the substantial increase in the amount of SCOD and total sugars, as shown in Table 2. All values were compared with those in the untreated SCG in order to conceive the effect of alkaline  $H_2O_2$  treatment. The concentration of SCOD and total sugars followed the same trend, whereby their augmentations were 555.96%, 594.92%, 706.73%, and 713.02% and 767.96%, 748.48%, 817.75%, and 793.94% for the 0.05%, 1%, 2%, and 4%  $H_2O_2$ -treated SCG, respectively, over the untreated SCG. Hence, SCOD solubilization and total sugar release increased with the increase in  $H_2O_2$  quantity. Pretreatment with 4% *w/w* hydrogen peroxide ( $H_2O_2$ ) resulted in the maximum increase in SCOD. This observation aligns with the findings of [31], who documented comparable effects in wheat straw treated with  $H_2O_2$  across different concentrations.

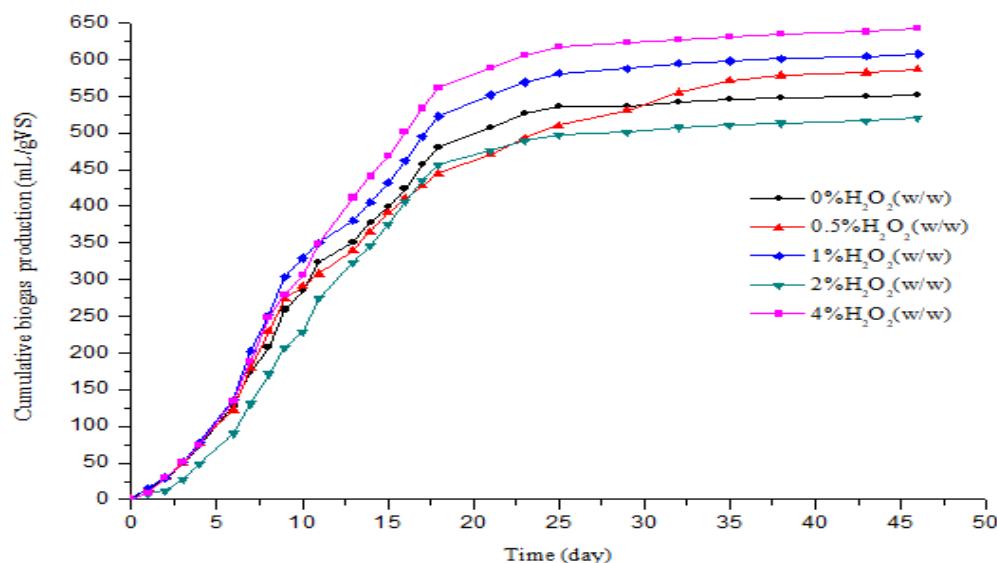
**Table 2.** Characteristics of SCG after  $H_2O_2$  pretreatment.

Parameters	Spent Coffee Grounds's Pretreatments				
	0%	0.5%	1%	2%	4%
Total solids (g/L)	22.06 ± 0.15	18.81 ± 1.57	16.47 ± 0.94	21.06 ± 2.97	17.54 ± 0.27
Total volatile solids (TVS) (g/L)	21.33 ± 0.16	18.17 ± 1.70	16.04 ± 0.91	20.95 ± 2.77	17.43 ± 0.34
% volatile solids (%)	96.73	96.52	97.41	98.84	99.39
Soluble chemical oxygen demand (SCOD) (go <sub>2</sub> /L)	13.59 ± 0.65	89.14 ± 4.94	94.43 ± 3.41	109.63 ± 0.89	110.48 ± 6.99
Total nitrogen Kjeldahl (TKN) (mg/g)	2.22 ± 0.13	2.02 ± 0.10	2.15 ± 0.28	2.08 ± 0.22	2.03 ± 0.16
Ammonium nitrogen (N-NH <sub>4</sub> <sup>+</sup> ) (mg/L)	1.00 ± 0.03	1.16 ± 0.02	1.17 ± 0.03	1.31 ± 0.02	1.1 ± 0.02
Protein (mg/g)	13.85 ± 0.60	12.59 ± 0.89	13.41 ± 1.74	13 ± 1.38	12.69 ± 1.00
Total alkalinity (mgCaCO <sub>3</sub> /L)	327.61 ± 8.45	354.76 ± 12.05	318.56 ± 10.08	257.02 ± 11.82	264.26 ± 9.97
Total soluble sugars mg/L	0.05 ± 0.00	0.40 ± 0.00	0.39 ± 0.00	0.42 ± 0.00	0.41 ± 0.00

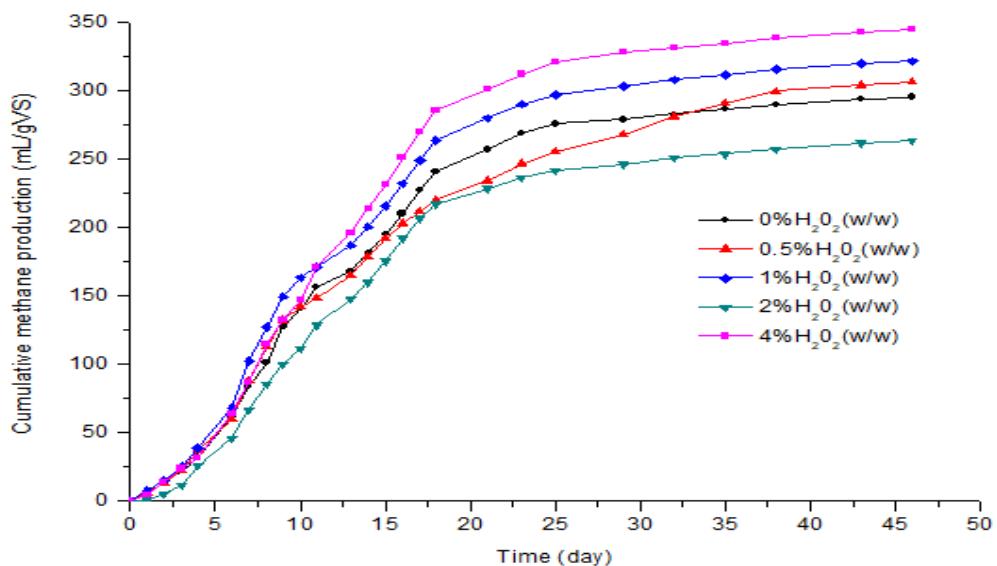
Consequently, the  $H_2O_2$  reagent was observed to break down the lignocellulose structure into readily biodegradable organic matter, which was then converted to a soluble phase and became available for digestion [3].

### 3.2. Effect of $H_2O_2$ Pretreatment on the Biogas and Methane Production

Batch anaerobic digestion assays were performed to investigate the feasibility of using  $H_2O_2$  pretreatment to enhance the anaerobic biodegradability of SCG. The cumulative biogas-methane production profiles are shown in Figures 1 and 2. Biogas-methane production is provided as the volume of biogas- $CH_4$  per mass of VS added. The untreated sample achieved 553 mL biogas/gVS, consistent with literature values [32]. However, the methane yield (295 mL  $CH_4$ /gVS, 53.76% of biogas) was lower than previously reported [32], possibly due to variations in SCG composition or digestion conditions.



**Figure 1.** Cumulative biogas of untreated and pretreated SCG.



**Figure 2.** Cumulative methane of untreated and pretreated SCG.

With the aim to verify the biogas- $CH_4$  yields detectable after  $H_2O_2$  oxidation, the samples pretreated by four  $H_2O_2$  loadings over the substrate solids (0.5, 1, 2, and 4%  $w/w$ ) were anaerobically digested in the same conditions of untreated SCG. After pretreatment, the highest biogas-methane production was 642.69 mL biogas/gVS and 345.53 mL  $CH_4$ /gVS with up to 16.28% and 16.93% improvements over the untreated SCG. It registered at a  $H_2O_2$  concentration of 4%  $H_2O_2$   $w/w$ . Although the 4%  $w/w$  hydrogen peroxide ( $H_2O_2$ ) pretreatment enhanced methane yield, this yield was lower compared to the results for

ultrasound pretreatment [33], and also lower than the results for 6% and 8% sodium hydroxide (NaOH) pretreatment [34]. Variations in SCG composition or experimental digestion conditions may account for these differences. However, it is important to consider that this study utilized  $H_2O_2$  pretreatment at ambient conditions (room temperature and pressure), potentially offering a more cost-effective approach compared to more energy-intensive pretreatments. The lowest biogas-methane values recorded were 520.37 mL biogas/gVS and 263.61 mL  $CH_4$ /gVS, which were 5.85% and 10.79% less than the untreated sample. It was obtained from SCG pretreated with a dosage of 2%  $H_2O_2$  *w/w*. The experimental outcomes for the biogas-methane potential test for 2%  $H_2O_2$  *w/w* pretreatment can likely be explained by the low alkalinity observed in this condition and the high quantity of ammonium nitrogen ( $N-NH_4^+$ ) (1.31 mg/L, with a 30.5% increment over the untreated SCG). The high concentration of hydrogen peroxide negatively influenced methane yields via the oxidation of degradation byproducts (VFA) necessary for anaerobic digestion [21]. The methanogens among the anaerobic microorganisms are likely the most affected by ammonia inhibition [30].

Although the increase in the magnitude of SCOD solubilization and total sugar release increased along with the increased  $H_2O_2$  concentration during the pretreatment and had the maximum values under these conditions, the escalation in the dosage of  $H_2O_2$  does not mean that the amount of biogas-methane generated followed the same trends. It is obvious that they behaved differently than the biogas-methane profiles.

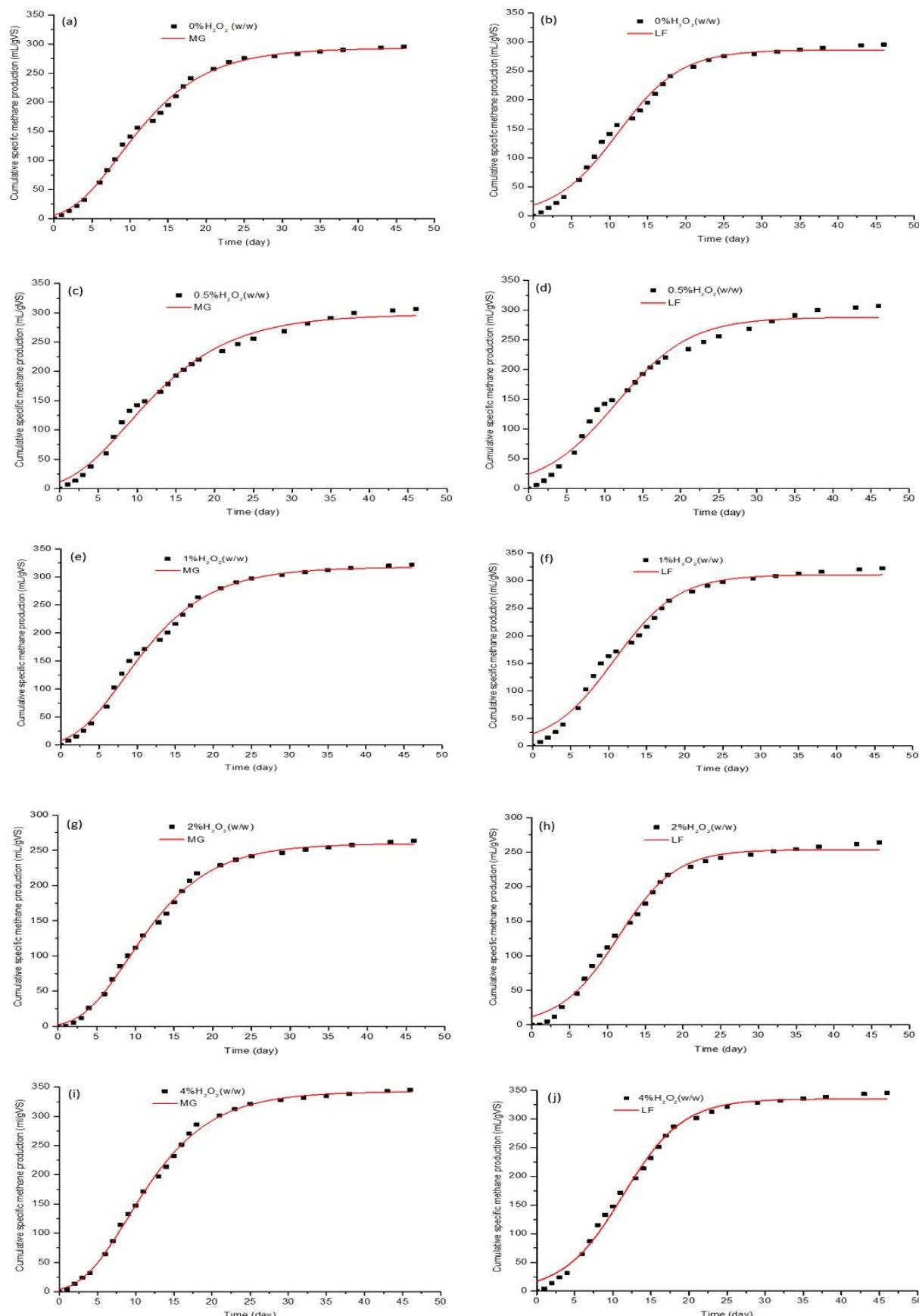
In this study, the optimum concentration of  $H_2O_2$  for enhanced biogas-methane production was found to be 4%  $H_2O_2$  *w/w*. Hence, the  $H_2O_2$  pretreatment used is attractive because it is more economical in terms of  $H_2O_2$  consumption.

### 3.3. Kinetic Study Results

The methane potential of substrates is important for the design and operation of biogas plants. Its determination is not always possible due to the long experimental time and lack of necessary infrastructure. Thus, kinetic models are adopted for the accurate prediction of methane potential [35]. In the present study, mathematical models were used to describe bacterial growth data and compare the effects of  $H_2O_2$  pretreatment on methane performance under different  $H_2O_2$  concentrations. The graphs of the cumulative methane production profiles depict a sigmoidal growth curve. Therefore, a modified Gompertz model and logistic function were adopted to simulate the experimental data of methane yields in the batch experiment and estimate the kinetic parameters (the duration of the lag phase ( $\lambda$ ), the maximum methane production rate ( $\mu_m$ ), and the methane production potential ( $A$ )).

The experimental cumulative methane yield and simulation results of the two models are shown in Figure 3. The obtained kinetic parameters and values of statistical indicators ( $R^2$  and root mean square error) for the studied kinetic models are summarized in Table 3.

The results showed that the kinetic parameters derived from the modified Gompertz model and the logistic function had similar relationships with untreated and pretreated SCG at different  $H_2O_2$  concentrations for both conditions (untreated and pretreated). The ultimate specific methane production value ( $A$ ) in the modified Gompertz model was higher than the logistic function value. Meanwhile, both values were lower than those obtained experimentally, and the models could not aptly predict the cumulative daily biogas yield data. The highest  $A$  in the two models was obtained in the 4%  $H_2O_2$  and 1%  $H_2O_2$  pretreatments, respectively, which suggested that  $H_2O_2$  pretreatment at the proper concentration could improve methane yields. The underestimated values of  $A$  using the modified Gompertz model and logistic function varied in a narrow range that is delimited between (0.85–3.15%) and (3.07–6.11%), respectively.



**Figure 3.** Experimental and simulated data obtained using modified Gompertz model (a,c,e,g,i) and logistic function model (b,d,f,h,j).

**Table 3.** Kinetic parameters estimated with modified Gompertz model and logistic function.

Model	Parameter	Treatment				
		0% $\text{H}_2\text{O}_2$ (w/w)	0.5% $\text{H}_2\text{O}_2$ (w/w)	1% $\text{H}_2\text{O}_2$ (w/w)	2% $\text{H}_2\text{O}_2$ (w/w)	4% $\text{H}_2\text{O}_2$ (w/w)
	A (mL/g VS)	292.990 $\pm$ 2.747	297.174 $\pm$ 4.970	317.332 $\pm$ 3.658	259.455 $\pm$ 2.040	342.510 $\pm$ 2.220
	$\mu m$ (mL/g VS/day)	17.221 $\pm$ 0.493	14.779 $\pm$ 0.658	18.667 $\pm$ 0.661	16.252 $\pm$ 0.408	21.065 $\pm$ 0.430
Modified Gompertz model	$\lambda$ (day)	2.315 $\pm$ 0.238	1.359 $\pm$ 0.423	1.906 $\pm$ 0.295	3.144 $\pm$ 0.197	2.958 $\pm$ 0.162
	$R^2$	0.996	0.991	0.994	0.998	0.998
	RMSE	6.223	10.016	8.393	4.728	5.105
	A (mL/g VS)	286.451 $\pm$ 4.236	288.052 $\pm$ 6.631	310.473 $\pm$ 5.325	253.589 $\pm$ 3.280	334.740 $\pm$ 3.797
	$\mu m$ (mL/g VS/day)	17.331 $\pm$ 0.884	14.861 $\pm$ 1.076	18.594 $\pm$ 1.107	16.611 $\pm$ 0.767	21.485 $\pm$ 0.862
	$\lambda$ (day)	2.8478 $\pm$ 0.456	1.860 $\pm$ 0.744	2.351 $\pm$ 0.539	3.770 $\pm$ 0.383	3.572 $\pm$ 0.339
Logistic Function model	$R^2$	0.989	0.975	0.984	0.992	0.994
	RMSE	11.003	15.926	13.917	8.702	10.016

Based on the maximum reaction rate ( $\mu m$ ), Li et al. (2015) [26] reported that under mesophilic conditions, acidogenesis and hydrolysis were found to be the rate-limiting steps for the anaerobic digestion of coffee grounds. As illustrated in Table 3, the estimated  $\mu m$  values from the two models vary in a narrow range: from 14.78 to 21.06 for the modified Gompertz model and from 14.87 to 21.49 for the logistic function.

According to [36], the  $\mu m$  shows a negative correlation with volatile solid (VS) content. In our study, the highest  $\mu m$  was obtained at 1% and 4%  $\text{H}_2\text{O}_2$  pretreatments in the two models, where volatile solids were found to be the lowest, whereas the lowest  $\mu m$  was obtained in the 0.5%  $\text{H}_2\text{O}_2$  pretreatment, and the time needed to reach its maximum methane production potential was long compared to other experiments. Furthermore, anaerobic digestion of SCG in the 0.5%  $\text{H}_2\text{O}_2$  pretreatment had considerable methane production and the shortest lag phase ( $\lambda$ ), presumably due to the good buffering capacity (354.76 mg  $\text{CaCO}_3$ /L) at this  $\text{H}_2\text{O}_2$  dosage in front of the high solubilization of degradable materials, which could shorten the acclimation time and enhance the adaptation ability of microorganisms. Consequently, the higher methane yield generated from the short lag phase indicated a fast adaptation of methanogenic bacteria to the substrate, which was consistent with the findings of [37]. As mentioned by [28], the correlation coefficient  $R^2$  is a measure of the strength of the relationship between measured and predicted values of methane yield [38].

From the results reported in Table 3, the correlation coefficient  $R^2$  values resulted in a fitting procedure using the modified Gompertz model, which varied within the range of 0.991–0.998, whereas the logistic function showed  $R^2$  values ranging between 0.977 and 0.993. Hence, the  $R^2$  values for the two models were all above 0.97, indicating that they could both be used for the kinetic simulation of anaerobic digestion of untreated and pretreated SCG.

The root mean square error (RMSE) results represent the deviation between predicted and measured data [39]. From Table 3, the RMSE ranged between 4.728 and 10.015 in the modified Gompertz model. Meanwhile, they ranged between 8.702 and 15.926 for logistic function.

The highest  $R^2$  and lowest RMSE were noted for the modified Gompertz model. The logistic model aptly predicts the experimental results in all conditions. However, the modified Gompertz model was more accurate in terms of fitting and predicting the methane yield in the same conditions. Consequently, the modified Gompertz model is recommended as the most suitable model for fitting cumulative methane yield in our tests.

#### 4. Conclusions

The biogas-methane potential of pretreated and untreated SCG was tested in anaerobic digestion. The results indicated that the  $H_2O_2$  pretreatment induced a significant increase in SCOD and total sugar leakage into the soluble phase in the range of 555.96–713.02% and 748.48–817.75%, respectively. However, this increment does not efficiently boost the biogas-methane enhancement in the same trend. It is obvious that they behaved differently than the biogas-methane profiles. The pretreatment of SCG gave negative results for the concentration of 2%  $H_2O_2$  *w/w*, and it also gave lower biogas-methane production volumes: 520.37 mL biogas/gVS and 263.61 mL  $CH_4$ /gVS. Our findings revealed that an  $H_2O_2$  concentration of 4%  $H_2O_2$  *w/w* was found to be the optimal condition for the enhancement of methane production. Under these conditions, the biogas-methane yielded a production of 642.69 mL biogas/gVS and 342.51 mL  $CH_4$ /gVS, which was 16.28% and 16.93% higher than the untreated SCG.

Moreover, this work confirmed the convenience of kinetic models in estimating and comparing kinetic parameters of the AD process and proved the appropriate fit of the experimental results to the proposed model. The modified Gompertz model was found to better simulate the experimental data of cumulative methane production than the logistic function across all experimental conditions, and this result confirms that the modified Gompertz model can be successfully used to predict methane production from untreated and oxidatively pretreated SCG.

Finally, all the experimental and numerical findings obtained from this work are useful to encourage the use of an integrated system composed of a chemical oxidative treatment followed by an AD process to treat SCG.

**Author Contributions:** Conceptualization, S.S., A.B. and K.D.; methodology, S.S., A.P. and K.D.; formal analysis, L.P and A.P.; investigation, S.S. and M.F.; data curation, F.P., A.B., K.D. and A.P.; writing—original draft preparation, L.P., A.B., K.D. and A.P.; writing—review and editing, S.S., K.D., A.B. and F.P.; supervision, K.D., M.F. and A.P.; project administration, K.D. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research received no external funding.

**Institutional Review Board Statement:** Not applicable.

**Informed Consent Statement:** Not applicable.

**Data Availability Statement:** The data that support the findings of this study are available upon request from the corresponding author.

**Acknowledgments:** This work was supported by the University of Constantine 3 (Algeria) and National polytechnic School of Constantine (Algeria).

**Conflicts of Interest:** The authors declare no conflict of interest.

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