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Article

Anaerobic Digestion and Biogas Potential: Simulation of Lab and Industrial-Scale Processes

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Abstract: In this study, a simulation was carried out using BioWin 3.1 to test the capability of the software to predict the biogas potential for two different anaerobic systems. The two scenarios included: (1) a laboratory-scale batch reactor; and (2) an industrial-scale anaerobic continuous lagoon digester. The measured data related to the operating conditions, the reactor design parameters and the chemical properties of influent wastewater were entered into BioWin. A sensitivity analysis was carried out to identify the sensitivity of the most important default parameters in the software's models. BioWin was then calibrated by matching the predicted data with measured data and used to simulate other parameters that were unmeasured or deemed uncertain. In addition, statistical analyses were carried out using evaluation indices, such as the coefficient of determination (*R*-squared), the correlation coefficient (*r*) and its significance (*p*-value), the general standard deviation (*SD*) and the Willmott index of agreement, to evaluate the agreement between the software prediction and the measured data. The results have shown that after calibration, BioWin can be used reliably to simulate both small-scale batch reactors and industrial-scale digesters with a mean absolute percentage error (MAPE) of less than 10% and very good values of the indexes. Furthermore, by changing the default parameters in BioWin, which is a way of calibrating the models in the software, as well, this may provide information about the performance of the digester. Furthermore, the results of this study showed there may be an over estimation for biogas generated from industrial-scale digesters. More sophisticated analytical devices may be required for reliable measurements of biogas quality and quantity.

Keywords: wastewater; anaerobic digestion (AD); biogas; BioWin; meat industry; simulation

1. Introduction

The production of biogas from covered anaerobic digesters is of growing interest to many developed and developing countries, as fossil-fuel resources decline [1,2]. Biogas is a renewable and sustainable energy, which is compatible with coal seam gas (CSG) and/or energy from crops, such as algae [3,4]. Despite the higher capital cost of covered anaerobic ponds when compared to uncovered ponds, covered anaerobic ponds offer significant advantages, such as odour control, intensification of the decomposition process, enhanced biological oxygen demand (BOD) removal, increase wastewater feeding rate, the potential for capturing methane-rich gas as a source for bioenergy and reduction in greenhouse gases (GHGs) [5]. While an anaerobic digester is a very useful element in a wastewater treatment plant (WWTP), anaerobic digestion (AD) is a very complicated chemical and biological process. It requires two to four months to start-up an anaerobic digester and an extra two to four months to analyse the efficiency of the process [6]. Monitoring the performance of anaerobic digesters requires a large dataset of measurements over extended time periods. The AD process requires a balance between the design parameters of the digester, the chemical and physical properties of the inlet wastewater, the conditions inside the digester and the biological aspects of the activated sludge. These variables have to be in the correct balance in order to accomplish optimum nutrient removal and economical biogas generation. Due to the complexity of this process, it is difficult in practical situations to apply these variables and, consequently, to identify problems that may affect the performance. Currently, especially in Australia, there are difficulties associated with covered anaerobic lagoons [7,8]. Some anaerobic digesters in the meat industry have been investigated, and it has been found that there is currently a lack of knowledge of anaerobic process regarding the design, operation and upgrading of these to covered anaerobic digesters. In many cases, in the Australian meat industry, despite much effort being made to measure biogas flow rate, the biogas quantity was unable to be accurately determined. This is due to many substantial technical problems, such as crust formation over the top of the anaerobic ponds/lagoons and a lack of design parameters [9,10]. The formation of the crust layer over the pond can lead to expensive damage to the pond's cover. This crust also illustrates the poor performance of the pond with regards to the wastewater treatment quality and quantity. This problem is not unique to one single abattoir and is a systemic problem in the red meat processing industry, which hinders the successful uptake of the technologies of covered anaerobic ponds [11]. Furthermore, there is uncertainty with regards to the quantity and quality of the recovered biogas. Thus, there is an urgent need for research in this area in order to investigate the feasibility of AD technology in meat industry wastewater treatment.

Modelling and simulation may help to reveal and interpret these problems and, at the same time, identify solutions [12–14]. It is important to be able to simulate the performance of an anaerobic digester during the design stage before any construction or modification begins. Modelling has previously been used to predict biogas production after calibration. In a study by Marcos *et al.* [15], modelling was used to simulate slaughterhouse wastewater effluent degradation and the methane generation rate after showing the accurate reproduction of the behaviour of an anaerobic digester. Modelling of the biogas production rate can also be used as an indication of the process performance [16]. In previous works by McCabe *et al.* [8], BioWin 3.1 software was used to simulate chemical oxygen demand (COD) removal and the subsequent biogas generation rate from two abattoirs, where crust (high content of fat, oil and grease (FOG)) accumulation was an issue. In those previous works, it was shown by using simulation that a large percentage of influent COD around 70% is not taking part in the AD process. BioWin was able to predict approximately the biogas production rate and the wastewater quality of the pond. This was impossible to do, due to the high accumulation of crust and the damage that occurred to the pond's cover. The simulation was able to provide a preliminary assessment of the pond performance and also the subsequent biogas production rate.

Due to the high complexity of AD processes, simulation can be an excellent tool for analysing, diagnosing and solving problems associated with these processes. This paper firstly provides some background information on the application of the BioWin computing modelling software for a number of studies. It then proceeds to report on the novel application of the software on two anaerobic systems, including: (1) a laboratory-scale batch reactor; and (2) an industrial-scale anaerobic lagoon digester. The purpose was to test the software for predicting the biogas potential for two vastly different scenarios. Two important parameters were used in carrying out the simulation: effluent COD content and the biogas generation rate. The effluent COD content of the wastewater was used to calibrate the software, and then, the calibrated software was used to predict the biogas generation rate over a long period of time. It has been found, by altering the BioWin default parameters, that BioWin is able to provide valuable information in regards to the efficiency of the anaerobic digester. Furthermore, BioWin can be used to overcome the uncertainty with regards to the amount of biogas produced, especially in pond/lagoon systems.

2. Background

As wastewater treatment models have evolved, there has been a natural progression to packaging of the models into software, as demonstrated by the early simulation work of Andrews and Graef in 1971 reported by Olsson *et al.* [17]. Nowadays, there are several simulator packages available on the market for wastewater treatment, such as Aquasim, BioWin, Simba, STOAT (Sewage Treatment Operation Analysis over Time) and WEST (Worldwide Engine for Simulation, Training and Automation). General purpose platforms, like MATLAB and Simulink, are frequently used for the simulation of wastewater treatment system control [17].

Simulation of the AD process can be carried out using software, such as BioWin. Activated sludge/anaerobic digestion models (ASDM) used by BioWin are recognized by the International Water Association (IWA), and these account for the most important parameters in treatment processes [18]. Much of the literature has addressed BioWin as an excellent tool for the design and analysis of WWTP. The recent setting of the default parameters in BioWin was studied by De Hass and Wentzel [19], and they showed that the recent default parameters are more realistic compared to the old versions. In one study by Elbeshbishy *et al.* [20], they achieved a good correlation of the experimental data with that predicted from BioWin while using the software's default kinetic and stoichiometric parameters. Furthermore, the calibrated software was able to predict most of the influent and effluent water fractions, such as COD, BOD, total suspended solids (TSS) and total Kjeldahl nitrogen (TKN). BioWin has been used to simulate large systems of wastewater treatment, which are combined with many elements, including anaerobic digesters [21]. Furthermore, BioWin was able to predict the biodegradability of organic compounds in the same order of the experimental finding [22]. In another study by Dhar *et al.* [23], however, all of the kinetic and stoichiometric parameters were kept at default values, except one: the hydrolysis rate. The methane production rate and volatile suspended solids (VSS) removal simulated by BioWin were in good agreement with the measured data. Studies have also reported the capability of BioWin to simulate other types of bioreactors successfully. A study by Eldyasti *et al.* [24] reported on the treatment of landfill leachate in a pilot-scale circulating fluidized bed reactor. This study illustrated that BioWin was able to accurately predict many major wastewater effluent parameters, such as TKN, ammonium nitrogen (NH_4-N), nitrate (NO_3-N), total phosphorus (TP), orthophosphate (PO_4-P), TSS and VSS with a mean absolute percentage error (MAPE) of 0%–20%. The study showed better accuracy using BioWin compared to other software. In that particular study, BioWin was calibrated by adjusting the wastewater fractions using measured experimental data. In another study by Hafez *et al.* [25], they showed that BioWin has the ability to predict biomass concentration in continuous stirred tank reactors (CSTR) with a MAPE of around 5%. Furthermore, the study demonstrated the ability to successfully predict many other parameters, among them the hydrogen production rate and the hydrogen yield compared to the measured data, with a MAPE of 4%. This has been done by calibrating the wastewater fractions included in BioWin and decoupling the solid retention time (SRT) from the hydraulic retention time (HRT). The trial and error method was used to achieve the best fit of the experimental data with that predicted by BioWin. It is obvious from the literature that BioWin can reliably be used as a design and analysis tool for WWTP, especially with suitable calibration. However, to my knowledge, BioWin has not been used to simulate industrial anaerobic ponds/lagoons (only by previous studies of the author) and/or at a lab-scale level.

BioWin software (EnviroSim Associates Ltd., Hamilton, ON, Canada) is easy to use, although it requires the user to have extensive knowledge and experience with wastewater treatment processes [26,27]. BioWin is a Windows-based computer simulation model developed by EnviroSim Associated Ltd. BioWin is capable of simulating the behaviour of AD systems by integrating biological and chemical processes to effectively determine biogas yield. The software contains two operational modules; a steady-state module and an interactive dynamic simulator. The steady-state module is used for simulating systems based on constant conditions, while the dynamic simulator allows the user to change time varying inputs or to the change operational strategy, which reflect real process conditions. BioWin has the ability to design simple and complicated WWTP [21,28,29]. Prediction of the behaviour of wastewater treatment systems, despite its complexity or the number of units included, becomes possible with BioWin simulation software. The dynamic behaviour of a wastewater system can be predicted under variable operation conditions and a wide range configuration of the process.

The BioWin ASDM model has fifty state variables and sixty process expressions. These expressions are used to describe the biological processes occurring in activated sludge and AD systems, several chemical precipitation reactions and the gas-liquid mass transfer behaviour for six gases. The model formulation requires pH determination. This complete model approach frees the user from having to map one model’s output to another model’s input, which significantly reduces the complexity of building full plant models, particularly those incorporating different treatment units.

3. Methodology

Firstly, the sensitivity of the parameters in the software was analysed in order to identify the impact of altering their values on the software's response. The parameters considered, based on the literature, are the hydrolysis rate (kinetic) and most of the wastewater fractions. Secondly, the software was calibrated based on methods reported in the literature. The calibration was done by altering some parameters to match measured data with those predicted by BioWin.

Finally, two examples with regards to simulation using BioWin 3.1 were presented: an industrial large-scale lagoon and a laboratory-scale reactor. This is to show the ability of BioWin to carry out the simulation for a diverse range of anaerobic digester designs and sizes. The simulation was based on two important parameters: the COD content of the effluent wastewater and the biogas generation rate. These examples were selected based on the availability of most of the important data required for the simulation.

3.1. Sensitivity Analysis

Sensitivity analysis is a technique that can be used to determine how different values of an independent variable will impact a particular dependent variable under a given set of assumptions. This technique is used within specific boundaries that will depend on one or more input variables, such as the effect that changes in hydrolysis rates will have on a COD outlet. Sensitivity analysis is a way to predict the outcome of a decision if a situation turns out to be different compared to the key prediction(s). Sensitivity analysis is very useful when attempting to determine the impact that the actual outcome of a particular variable will have if it differs from what was previously assumed. By creating a given set of scenarios, the analyst can determine how changes in one variable(s) will impact the target variable. In this study, the most important kinetic parameter (hydrolysis rate) and other wastewater fractions were tested to determine their impact on the output of BioWin. Figure 1 shows the impact of altering the value of the hydrolysis rate (AD) (the hydrolysis rate of particulate organics in anaerobic digesters, BioWin 3.1) parameter on the COD outlet from a digester. It is obvious that this parameter is highly sensitive, as it represents the limiting step in the degradation process. The other example is presented in Figure 2, this figure shows the impact of altering the unbiodegradable soluble COD in the wastewater on the COD outlet from the digester. The value of this parameter is between 0 and 1, and Figure 2 shows a very small effect of altering its value.

The sensitivity analyses carried out in this study have been summarized in Table 1. The table shows that both the hydrolysis rate (kinetic parameter) and Fbs (readily biodegradable (including acetate) gm COD/gm of total COD) are highly sensitive. These two parameters represent the limiting steps in the digestion process and the fraction of the wastewater that degrades first, respectively. In this present study, only the hydrolysis rate (AD) (the hydrolysis rate of particulate organics in anaerobic digesters, BioWin 3.1) was altered, due to the availability of information and its high sensitivity.

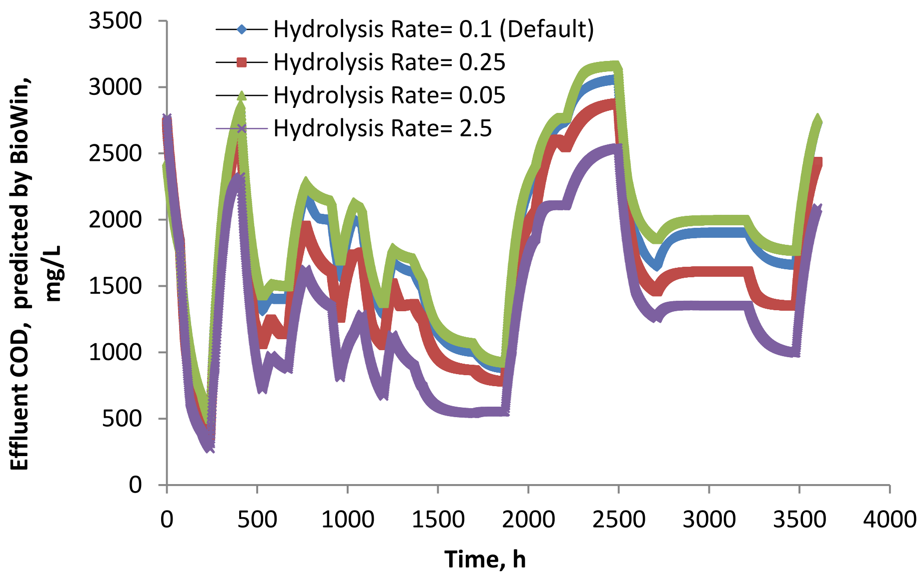

Figure 1. Predicted outlet chemical oxygen demand (COD) at different hydrolysis rates.

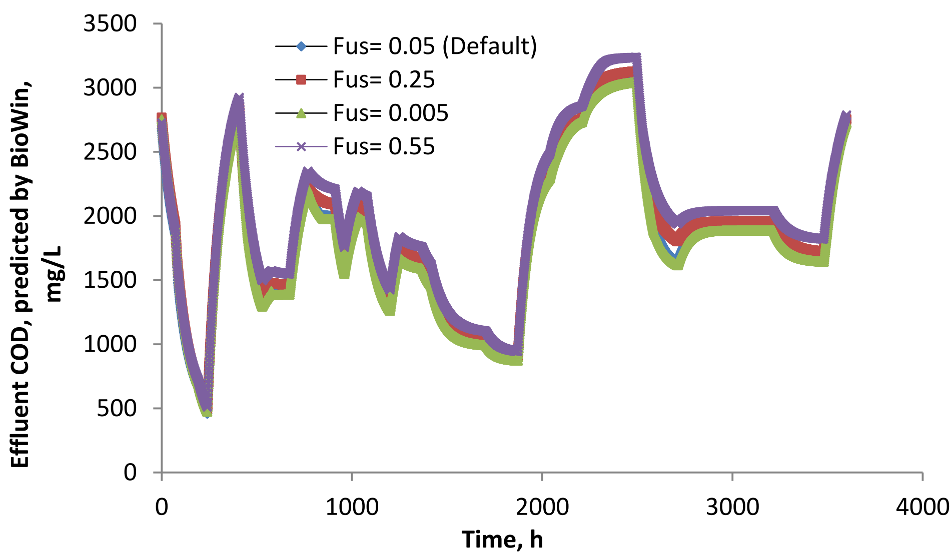

Figure 2. Predicted outlet COD at different Fus (unbiodegradable soluble gm COD/gm of total COD).

Table 1. Sensitivity analysis of the different parameters of the software. AD: anaerobic digestion.

Parameter	Description	Sensitivity
Kinetic, hydrolysis rate (AD)	1/day	High, limiting step
Wastewater fraction, Fus	Unbiodegradable soluble gm COD/gm of total COD	Low
Wastewater fraction, Fup	Unbiodegradable particle gm COD/gm of total COD	Low
Wastewater fraction, Fbs	Readily biodegradable (including acetate) gm COD/gm of total COD	High
Wastewater fraction, Fxp	Non-colloidal slowly biodegradable gm COD/gm of slowly degradable COD	Low
Wastewater fraction, Fac	Acetate gm COD/gm of readily biodegradable COD	Low
Operation, seed sludge age	In days	Low

3.2. Model Calibration Methods

In order to match effluent COD and biogas production rate values from an anaerobic digester with that predicted by BioWin, the following calibration actions took place. Many of these actions below have been suggested by the literature in order to match the result of BioWin with the measured data. Altering the default value of the hydrolysis rate (AD) (the hydrolysis rate of particulate organics in anaerobic digesters, BioWin 3.1) in the BioWin hypothetical digester is a good and reasonable option. Increasing the value of the hydrolysis rate means increasing the efficiency of the digester. This action will lead to the reduction of the effluent COD values. Hydrolysis is the first step in the reaction sequence during the digestion process and has been identified as the limiting step. It also represents the most important parameter in the matching process of experimentally measured data with BioWin predictions [23]. This action has been shown to be successful with regards to matching the results of the measured and predicted data of this study. Furthermore, this action provides information about the efficiency of the anaerobic digester.

In a study by Liwarska-Bizukojc *et al.* [28], they have illustrated that the value of COD in the effluent depended on the fraction of non-biodegradable soluble COD (Fus). The lower the fraction of Fus was, the lower the COD of the effluent. The total COD is a combination of readily biodegradable (Fbs), unbiodegradable soluble (Fus) and unbiodegradable particulate (Fup); the default values for these fractions are 0.16, 0.0001 and 0.13 g COD/g of total COD, respectively (the total should be less than 1). Changing these fractions by decreasing the unbiodegradable and increasing the biodegradable fractions should reduce the outlet COD. This action also means increasing the biodegradability of the materials entering the pond. In this study, it was not applicable to change the stoichiometry of the wastewater, such as Fus, Fbs and Fup, due to the non-availability of the influent COD characteristic. Although, when these values were altered from their default values, it was not sufficient to match the experimental data with the BioWin prediction. In our case, the only action that was able to match the measured and predicted data was the hydrolysis rate, which also showed high sensitivity.

3.3. Description of the Two Anaerobic Systems

3.3.1. Scenario 1: Industrial-Scale Anaerobic Continuous Lagoon

The measured data from the industrial-scale anaerobic lagoon (King Island covered lagoon, Tasmania, Australia) [30] were used for simulation purposes, due to the details provided with regards to the measured variables. This lagoon, relatively speaking, has formed a low crust during a long period of operation, which may indicate the high efficiency of the pre-treatment process. The plant is applying many pre-treatment processes for the wastewater before being directed to the lagoon, such as screening and diffuse air flotation (DAF). This may contributed to reducing FOG materials from flowing to the pond and, as a result, reduced problems associated with the process, at least over the first eight months. In the author's previous article [8], a reduction to the inlet COD of around 70% was applied in order to match the experimental data with that simulated by BioWin. This reduction in inlet COD was applied to two abattoirs in Queensland, Churchill and Southern meat [8,11]. This was a logical action due to the thick crust formed at the top of the ponds in these abattoirs, which measured around 1 m in some places of the ponds. This was justified by the fact that the floating materials, expected to be mostly fat, on the top of the pond are not contributing to the digestion process. For this reason, the COD content of the crust was eliminated from the simulation. The simulation in the case of King Island did not require any reduction to the COD content of the influent wastewater, due to the absence of such problem.

To mimic the actual conditions at the King Island covered lagoon, the simulation was carried out considering all of the events that happened and described in the report published by Meat Livestock Australia (MLA). These events were:

- Working days in the plant are 5 days;
- Plant shutdown happened from 5 to 16 April (no flow of wastewater to the lagoon);
- Temperature variation during the whole monitoring period;
- Change in the flow rate from 290 m^3/day to 350 m^3/day in late February.

The characteristics of the wastewater influent to the King Island covered anaerobic digester as described by MLA's final report [30] are shown in Table 2. The data in Table 1 were fed to BioWin to carry out a dynamic simulation.

Table 2. Characteristics of the wastewater fed to the covered anaerobic pond at King Island. TKN: total Kjeldahl nitrogen; TP: total phosphorus; and DO: dissolved oxygen.

Parameter	Unit	Mean values for different periods over 30 days				Comments
		15 December 2011–24 February 2012	27 February–4 April 2012	Shut down 5–16 April 2012	17 April–5 July 2012	Every Saturday and Sunday
Flow rate	m^3/day	290	350	0	350	0
Total COD	mg COD/L	2200–7800	2200–7400	0	1600–5500	0
TKN	mgN/L	130–350	150–450	0	130–450	0
TP	mgP/L	23	23	0	23	0
Nitrate N	mgN/L	0	0	0	0	0
pH	-	8.39–6.97	8.26–6.7	0	6.93–8.68	0
Alkalinity	mmol/L	13	13	0	13	0
ISS *	mgs/L	200	200	0	200	0
Ca	mg/L	115	115	0	115	0
Mg	mg/L	20	20	0	20	0
DO	mg/L	0	0	0	0	0

* Inorganic suspended solid, assumed, due to the lack of measurements, the sensitivity of this parameter was found to be very low and to have a minimum effect on the prediction of BioWin.

Table 3 illustrates the specifications of the lagoon operation conditions, such as volume, temperature and depth.

Table 3. King Island anaerobic digester specifications.

Parameters	Unit	Value
Volume	m^3	2700
Depth	m	5
Temperature	°C	14.4–43.1

3.3.2. Scenario 2: Laboratory-Scale Batch Reactor

A batch reactor, reported by Petruy and Lettinga [9], was used to measure both COD reduction (%) and the methane generation rate (mL/h) over 700 and 6 h, respectively. The digester, as explained in the article, is a glass expanded granular sludge bed (EGSB), batch reactor, closed circuit, with a total volume of 2.4 L. Granular sludge of 6.35 g VSS/L was used as the inoculum.

The batch process was simulated using BioWin software by uploading the characteristics of the inlet wastewater into the hypothetical digester created by BioWin with a very high retention time. The flow to the reactor was kept at a specific rate for a period of time sufficient to fill the rector volume, then switched to zero for the rest of the time. The flow rate was chosen as 0.0024 m^3/day (2.4 L/day) to make sure that the reactor will be full at the end of that day (the reactor volume is 2.4 L). The default value of the hydrolysis rate (0.1) was altered to 0.01 (1/day); this value has been provided by the article, as it was estimated from experimental measurements.

Table 4 presents the characteristic of the wastewater and the way it was introduced to the hypothetical batch reactor; the table is organized based on the requirements of BioWin software. As can be seen in Table 4, the feeding time to the hypothetical digester continued for 1 day, and then, the feeding was stopped over the remaining 29 days.

Table 4. Characteristics of the wastewater fed to the batch anaerobic reactor in the Petruy and Lettinga experiment [9].

Time (day)	Flow rate (m^3/day)	TCOD (mg COD/L)	TKN (mg N/L)	TP (mg P/L)	Nitrate N (mg N/L)	pH	Alkalinity (mmol/L)	ISS (mg SS/L)	Ca (mg/L)	Mg (mg/L)	DO (mg/L)
1	0.0024	2700	280	38.6	55	7	4.86	45	80	15	0
2	0	0	0	0	0	0	0	0	0	0	0
--	0	0	0	0	0	0	0	0	0	0	0
--	0	0	0	0	0	0	0	0	0	0	0
30	0	0	0	0	0	0	0	0	0	0	0

Table 5 illustrates the design parameters of the actual batch digester with regards to the volume and the depth of the reactor and the operation temperature. The temperature was controlled and kept at 30 ℃ over the entire period of the actual experiment. Same parameters and the temperature have been applied in the hypothetical digester.

Table 5. Batch anaerobic digester specifications.

Parameters	Unit	Value
Volume	m^3	0.0024
Depth	m	1.07
Temperature	℃	30

4. Results and Discussions

4.1. Scenario 1: Industrial-Scale Continues Lagoon

Many assumptions have been made in order to carry out the simulation for the anaerobic lagoon. The lagoon was assumed as a continuous bio-reactor due to the high flow rate of the influent wastewater. One of BioWin default values in the kinetic parameters' list was adjusted due to some statements in the report and for calibration purposes. The default value of hydrolysis was altered to 0.05 (1/day) for the period from 5 December 2011 to 24 May 2012, and 0.4 (1/day) for the rest of the period, *i.e.*, till 5 July 2012. The default value of hydrolysis in BioWin is 0.1 (1/day). The altering of the hydrolysis rate was significant to accomplish a match between the measured values of the effluent COD and that predicted by BioWin. The report has illustrated an efficiency of COD removal of approximately 50% during the period from the start till 21 May 2012. This reduction in COD was attributed to the dilution of the influent wastewater by low strength water initially present in the pond [30]. The hydrolysis of 0.4 (1/day) was applied due to a claim in the report of a high improvement in the performance of the digester after 21 May 2012, due to a shock load. The average COD loading to the pond has decreased from 5000 mg/L to 3500 mg/L, as shown in Table 2. This may justify increasing the value of the hydrolysis rate. Figure 3 clearly illustrates the improvement in the digester efficiency, due to the decline in the ratio of volatile fatty acid to total alkalinity (VFA/TA), this starting approximately on 30 April 2012. To determine pond stability from alkalinity and VFA accumulations, two common calculations can be applied; a weight ratio of VFA:TA of 0.25–0.35:1 is indicative of a healthy pond system [31], alternatively, a molar ratio of TA:VFA greater than or equal to 1.4:1 should be maintained for a stable and well-buffered system. Furthermore, the stability of this ratio is more important than the magnitude [32]. As can be seen in Figure 3, the ration of VFA:TA starts to decline sharply below 0.6:1 after 30 April 2012, which clearly indicates an improvement of the biological activities in the lagoon.

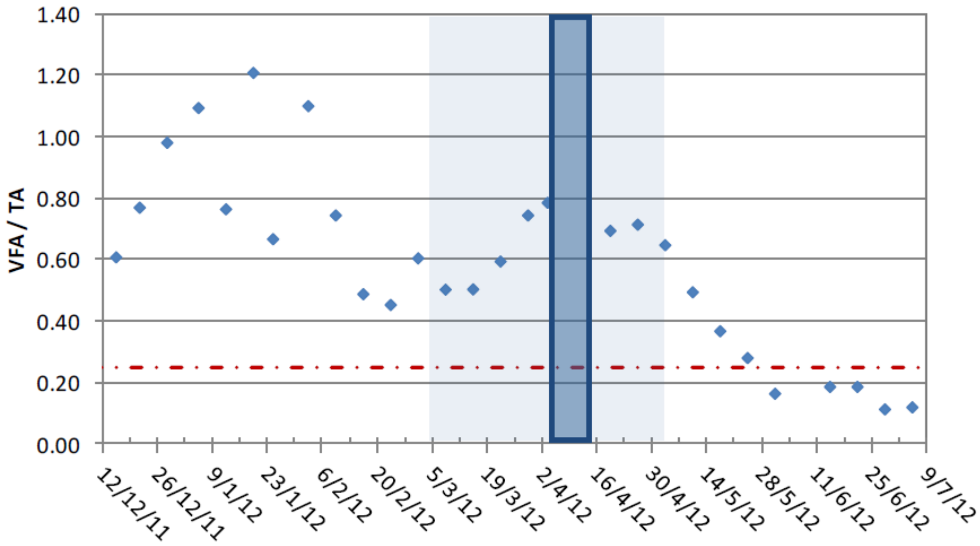

Figure 3. Ratio of volatile fatty acid to total alkalinity (VFA/TA) over the entire monitoring period [30]. Copyright 2013 by the Rural Industries Research and Development Corporation, Australia.

Figure 4 illustrates a comparison between the measured effluent COD from the lagoon at King Island and that predicted by BioWin. The trends of these two data match very well with a MAPE less than 15%. Figure 4 illustrates that BioWin is able, to a large extent, to simulate the COD outlet from the pond over a long period of time, over seven months.

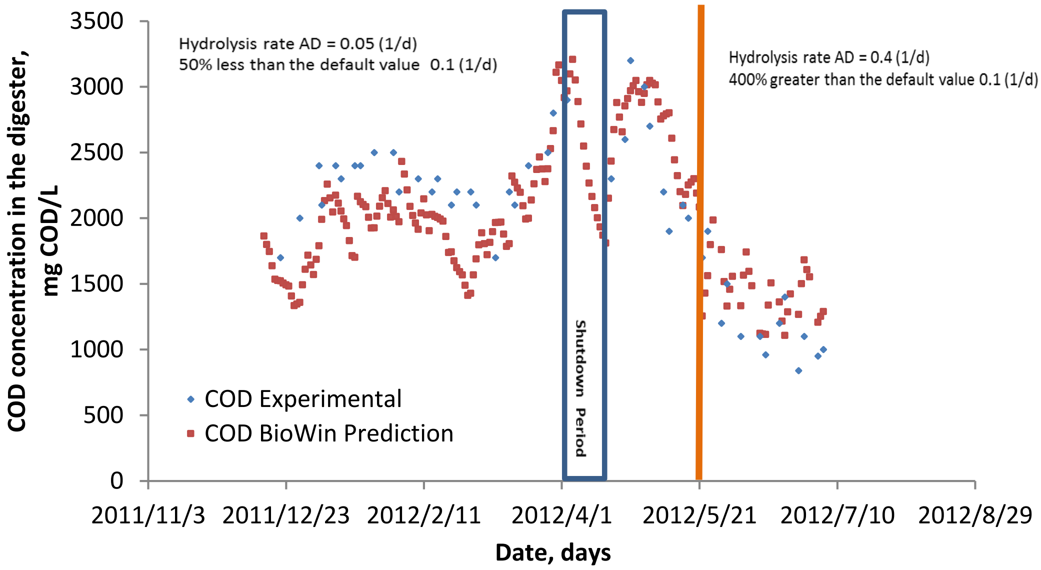

Figure 4. Measured outlet COD *vs.* BioWin predictions at two stages before and after the shutdown of the digester.

To confirm the match between these data, the coefficient of determination (*R*-squared) was determined. Figure 5 shows the *R*-squared value of the measured and predicted data. The *R*-squared value is around 61%, which may be reasonable and acceptable in vigorous and complex environments, such as AD process. Furthermore, the low *R*-squared value may be due to the long simulation period and the large number of data considered. Due to the high complexity of the process and as stated by other researchers [8,28], a MAPE for the measured and predicted data of 7% to 15% is sufficient for the indication of the correct dynamic calibration.

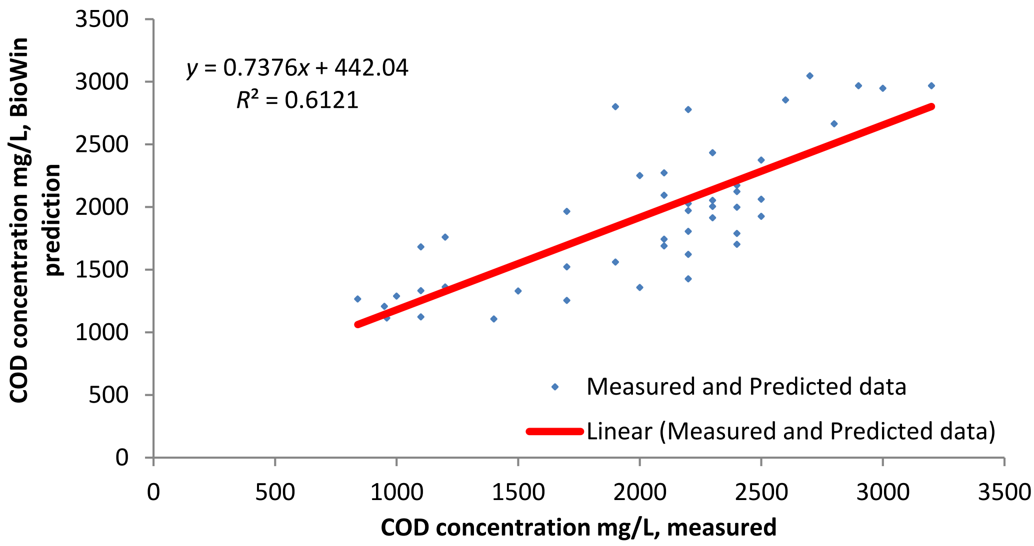

Figure 5. *R*-squared of the measured outlet COD *vs.* BioWin predictions.

Figure 6 is a comparison between the measured biogas production from the King Island anaerobic digester and that of the predicted hypothetical digester created by the BioWin software. This figure illustrates that although the BioWin prediction did not match the measured biogas generation rate, it followed the measured trend quite well. The difference between the measured and predicted data is approximately a factor of 2.5. In other words, the measured data of biogas are higher than those predicted by a factor of 2.5.

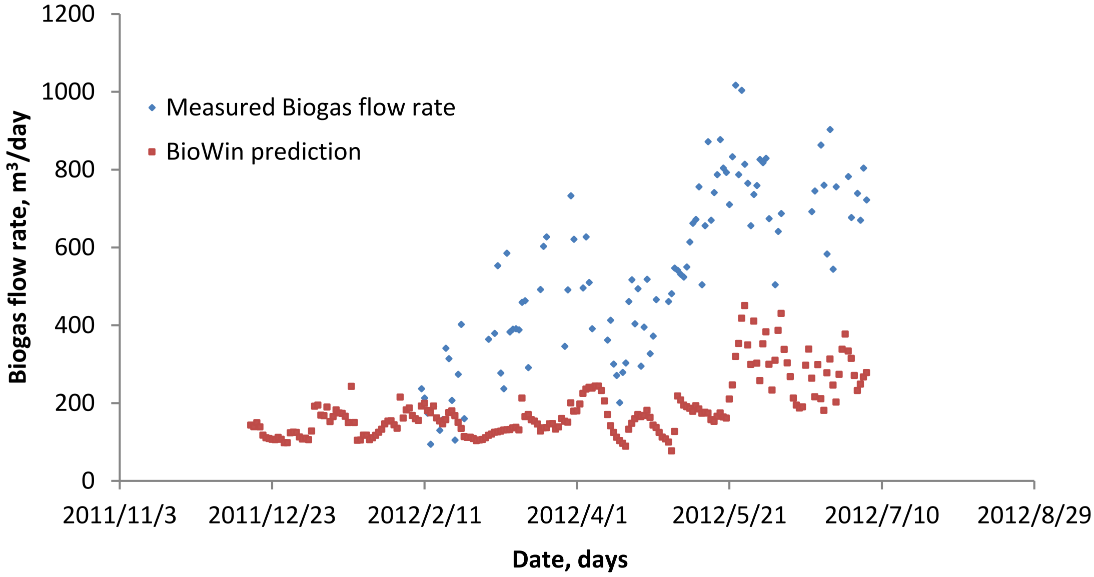

Figure 6. Comparison between the measured biogas from the King Island plant *vs.* that predicted by the BioWin.

As can be seen in Figure 7, a good match can be achieved when the predicted data were multiplied by a factor of 2.5. Figure 7 also shows two lines that represent the average biogas generated by both the actual and the hypothetical digesters. The measured average biogas generated by the lagoon is around 516 m^3/day and that predicted by BioWin is around 460 m^3/day. These results contribute to a MAPE of less than 11%, which indicates a good match of the data. The coefficient of determination value for the measured and predicted biogas flow rate was estimated to be around 0.46. This low value may be attributed to the large number of data considered, around 135 points. The agreement of the model prediction and the measured data has been explored in more detail in Section 5 using other indices of evaluation.

The 2.5-times difference between the experimental and measured data is attributed to the conditions at the lagoon and the measuring device. The report has mentioned a great discrepancy in the biogas quantity and quality measurement due to high moisture content, temperature fluctuation and the effects of rain on the lagoon [30]. The high moisture content of the biogas may be related to the large surface area of the pond (50 m × 26 m) and the pond temperature, which approaches 43 °C on many occasions. This may affect the performance of the measuring device, thus explaining the high discrepancy between the measured and predicted data. Instruments, such as flow meters, measure the total flow regardless of the composition. In contrast, BioWin does not consider moisture content in the biogas composition. This leads to the conclusion that the discrepancy may be attributed mainly to the high moisture content of the biogas mixture.

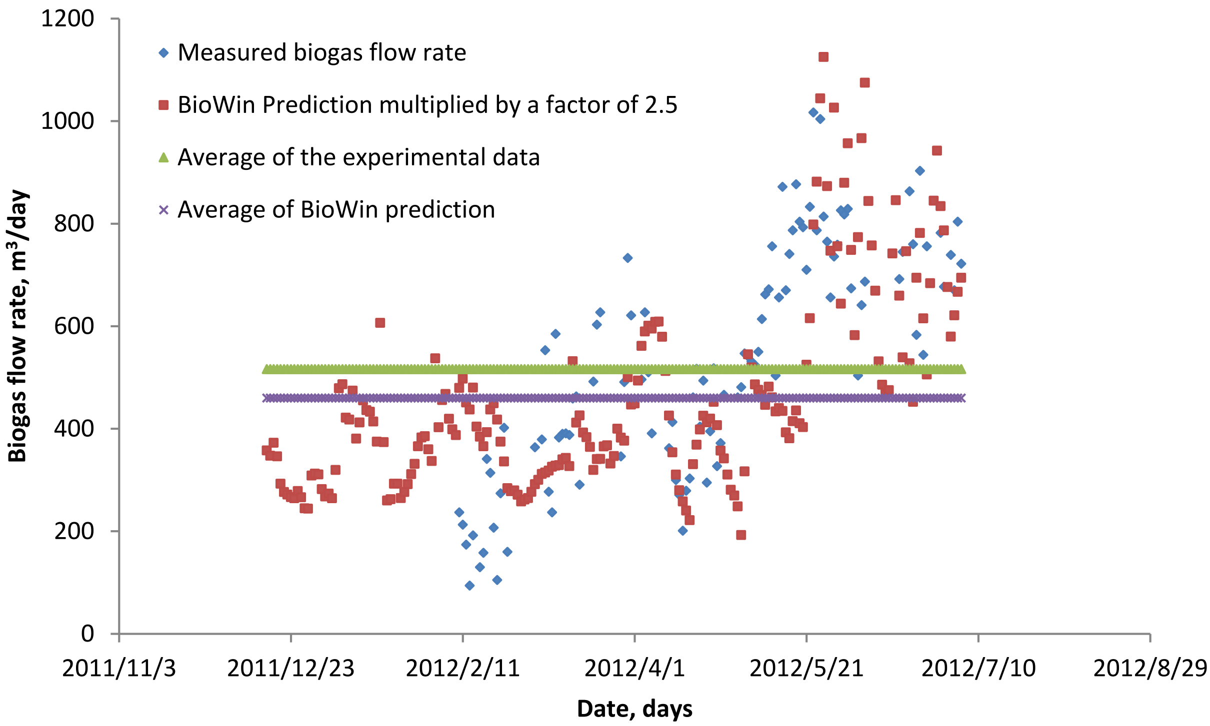

Figure 7. Comparison between the measured biogas from the King Island plant *vs.* that predicted by the BioWin multiplied by 2.5.

The uncertainty with regards to the quantity of the generated biogas reported in many publications [8], especially in the meat industry, makes BioWin a useful tool to forecast such data. In this study, BioWin has shown its ability to predict un-measured data after calibrating these with reliable measured data. Furthermore, it was able to analyse the efficiency and performance of an industrial-scale digester through manipulating its default parameters. The next step is to confirm BioWin's ability to simulate a lab-scale digester.

4.2. Scenario 2: Laboratory-Scale Batch Reactor

Figure 8 shows a comparison between the measured COD reduction (%) and that predicted by the BioWin software. The figure clearly illustrates a good match of the measured and predicted data with a MAPE of slightly above 7%. The experimental data show that the reduction in the COD content of the digester has declined by 70% during the first few hours. The COD then smoothly reduces to approximately 88% along the next 200 h and continues at this level along the remaining time of the experiment. In contrast, the simulated data show a sharp reduction in the COD content of the digester to around 90% during the first 50 h. This slight discrepancy in the early prediction of BioWin may be explained by the lack of information with regards to some parameters. Some assumptions were made in regards to the characteristic of the wastewater, such as its content of inorganic suspended solids (ISS), magnesium (Mg) and calcium (Ca). Furthermore, the pH and alkalinity of the influent wastewater and/or the digester are important to be monitored and fed into BioWin in a continuous mode. A sensitivity analysis was carried out for these parameters, and this showed that large changes in the values can alter the prediction of BioWin by 10%–20%, which is sufficient to enhance the matching between the predicted and measured data.

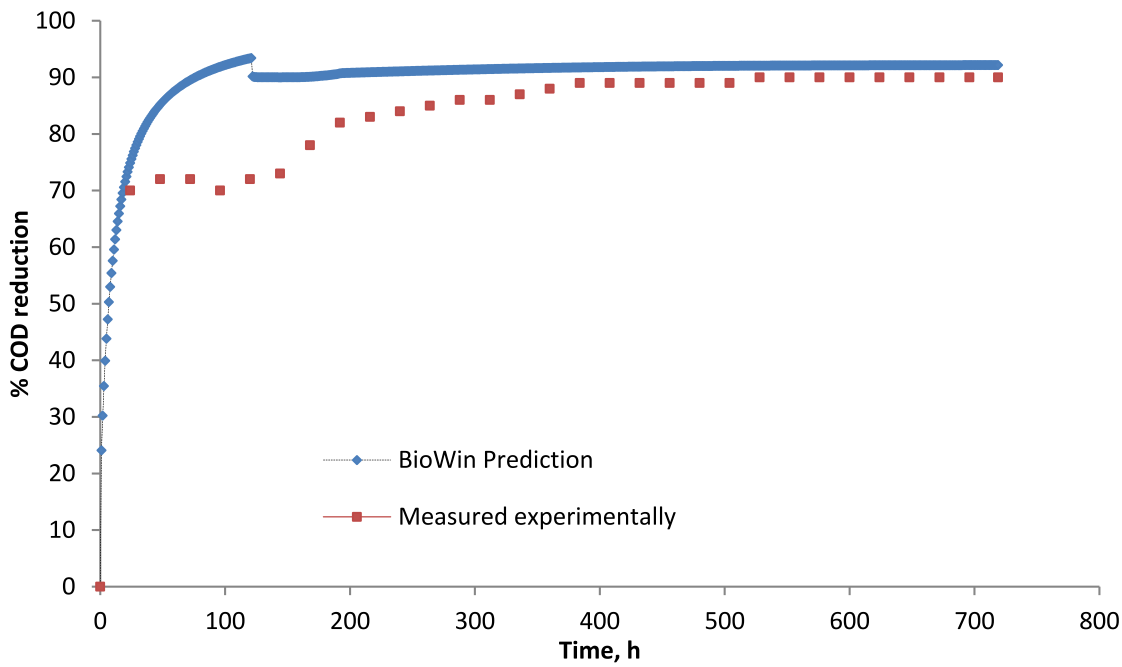

Figure 8. Fractions of COD eliminated during a period of 30 days; a comparison between BioWin prediction and experimental measurement; mean absolute percentage error (MAPE) = 7.1%.

To confirm the good matching of the measured and the predicted data, the quality of the fit of these data was expressed by the coefficient of determination (*R*-squared). *R*-squared indicates how much of the observed variability in the data was accounted for by the simulation. An *R*-squared value of around 87.5% is estimated, which indicates an adequate agreement between the experimental data and the data obtained by the simulation. It is clear that using experimentally-measured kinetic parameters in the software instead of the default values, especially the hydrolysis rate, is sufficient to calibrate the software and give a good prediction.

The second step in the simulation, after matching the measured COD content of the actual reactor with that predicted by BioWin over the entire period of the experiment, is to use the calibrated software to predict the biogas generation rate. The article by Petruy and Lettinga [9] has provided the methane generation rate in mL/h over 6 h only. Furthermore, the data were linearized by drawing a line between the measured values. In our study, BioWin was first used to predict the methane production rate over the entire period of 30 days, as shown in Figure 9. It is obvious from the figure that the methane generation rate increases sharply after 180 h from starting the experiment to a value around of 17 mL/h. Additionally, this is only for a short time, for 5 h, where the methane production rate rises from 17 mL/h to 170 mL/h and then declines to around 20 mL/h. After this decline, the reduction in the methane generation rate follows a smooth trend until it reaches zero. To explain this behaviour of methane production in an anaerobic digester, the accumulation of methane over the entire experimental period was plotted, as shown in Figure 10. In a study by Esposito *et al.* [33], they showed that the cumulative bio-methane production curves are usually either reverse L-shaped or S-shaped. In the reverse L-shaped graphs, as in this case (Figure 10), the initial phase is distinguished by a higher methane generation rate that progressively decreases during the intermediate phase up to tending toward zero at the end of the final phase. In the S-shaped graph, similar to reverse L-shaped graph, the initial phase is distinguished by a high methane generation rate, but lower than the one characterizing the intermediate phase, whereas during the final phase, similar to the reverse L-shaped graph, the methane generation rate tends to zero. Figure 10 shows that methane accumulation can reach a value of 1800 mL at the end of the experiment, in this case 30 days.

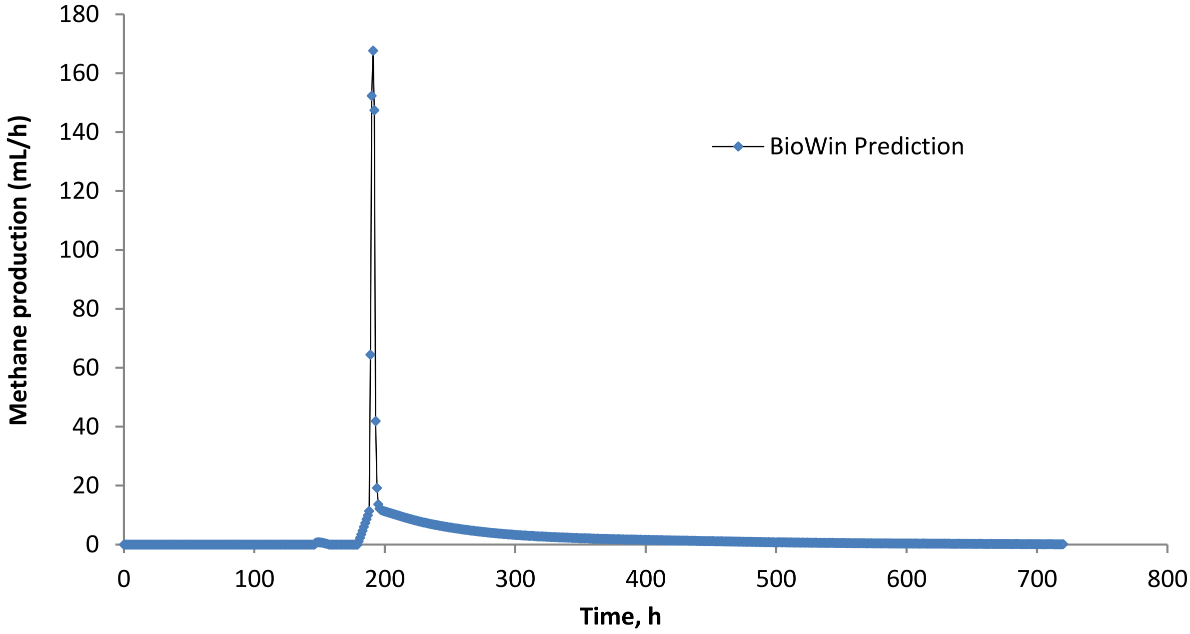

Figure 9. Methane production (mL/h) with time for a period of 30 days, predicted by BioWin for a batch laboratory anaerobic reactor (volume: 2.5 L).

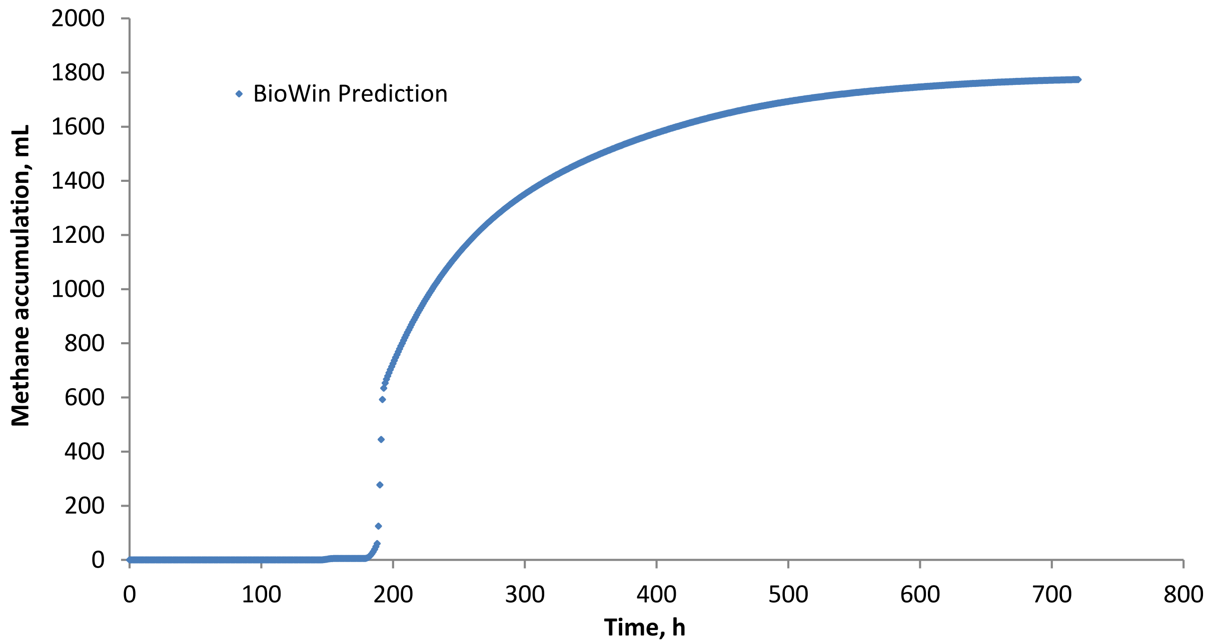

Figure 10. Methane accumulation (mL) with time for the entire period of the experiment as predicted by BioWin.

The value of the accumulated methane in the study of Petruy and Lettinga [9] has been given over 6 h only. The experimental methane accumulation curve begins with a methane volume of 20 mL.

For the purpose of comparison, this was compared to methane accumulation in millilitres over a 6-h period from the simulation. The 6 h from the simulation were selected based on a starting point approximately close to 20 mL. Figure 11 shows a comparison between the measured accumulated methane over the 6-h period and the BioWin prediction. To illustrate the matching between the predicted and the measured data, the coefficient of determination (*R*-squared) was estimated. An *R*-squared value over 80% was estimated, which indicates an adequate agreement between the experimental measurements and the data obtained from the simulation. It is not clear what the reason was for considering only 6 h of methane accumulation in the study by Petruy and Lettinga [9]. This analysis again shows that BioWin can be a good tool for predicting both the quality of the effluent and the generated quantity of biogas, even with small lab-scale experiments. It is worth mentioning that the greatest impact on BioWin prediction accuracy comes from feeding it with accurate data, specifically with regards to the influent characteristic and the kinetic parameters (such as the hydrolysis rate).

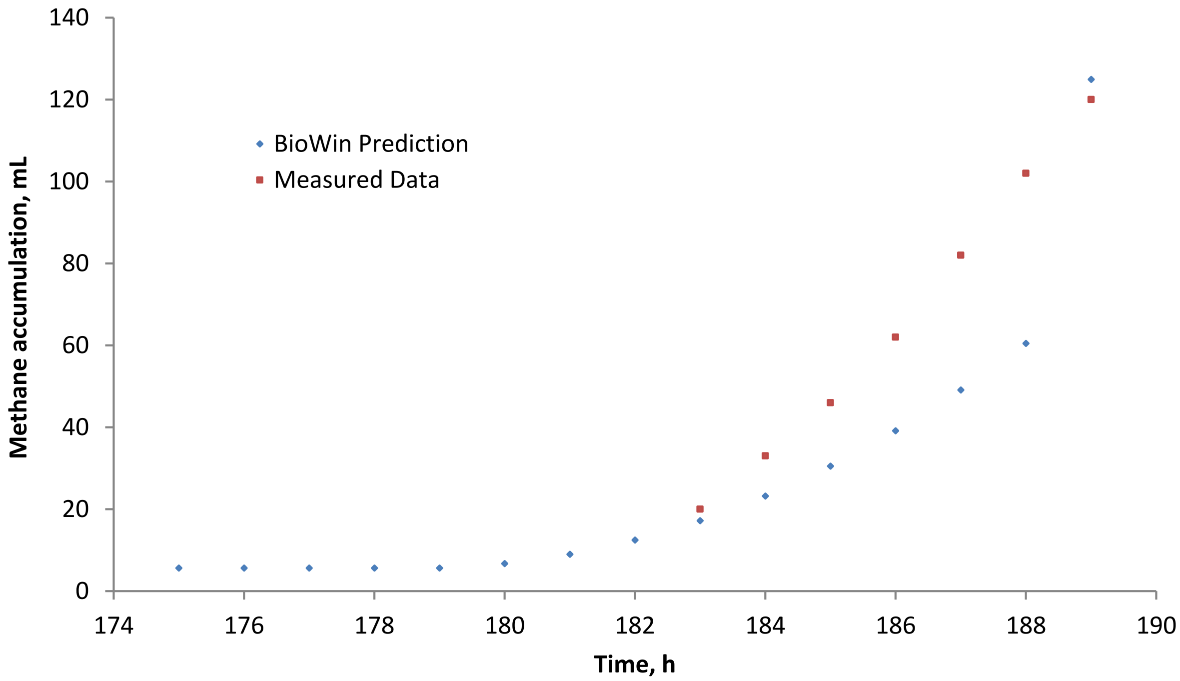

Figure 11. Methane accumulation (mL) with time for a period of 6 h; a comparison between the BioWin prediction and experimental measurement.

5. Statistical Analysis of Agreement

A statistical analysis was carried out using different techniques in order to evaluate the agreement between the measured and predicted data. The methods applied were the coefficient of determination (R^2), the correlation coefficient (r) and its significance (p), the general standard deviation (SD) and the Willmott index of agreement. The results of this statistical analysis are presented in Table 6. The results shows that the correlation coefficient (r) for the measured and predicted data are significant ($p < 0.05$). This means that the number of data involved in the evaluation of the model is sufficient and that the results are significant in all cases. The lowest correlation coefficient is around 0.66, and the lowest Willmott index of evaluation is around 0.85. All of these results illustrate a good match between the measured and predicted data.

Table 6. Different indexes of evaluation for the model prediction.

Data	**Number of points**	***R*-squared**	***r***	***p***	**Willmott index of agreement**
Figure 3	48	0.61	0.78	0.0001	0.85
Figure 6	135	0.46	0.66	0.0001	0.996
Figure 8	30	0.88	0.997	0.0001	0.999
Figure 11	7	0.81	0.98	0.0001	0.999

The other methods used to evaluate the agreement between the measured and predicted data are through estimating the mean and the standard deviation values of the sets of data. Table 7 demonstrates that the mean value of each set of measured data and that predicted by BioWin are very close. Similar results are shown for the standard deviation values. The MAPEs for each predicted and measured mean and *SD* values were estimated, and the results are shown in Table 6. The table shows the *SD* for the calculated MAPEs of 6.3% to 21.6%, which confirms the good agreement.

Table 7. Mean and standard deviation (*SD*) for the measured and predicted data.

Data	**Number of points**	**Measured**		**Predicted**		**MAPE**	
		Mean	***SD***	**Mean**	***SD***	**Mean**	***SD***
Figure 3	48	2067.70	631.43	1917.96	538.42	7.2	14.7
Figure 6	135	572.16	211.35	557.52	224.67	2.5	6.3
Figure 8	30	82.06	9.21	88.35	9.56	7.6	3.8
Figure 11	7	66.4	36.72	62.41	44.66	6.0	21.6

6. Conclusions

In this study, the simulation of both an industrial covered anaerobic lagoon and a lab-scale batch rector has demonstrated that simulation can be carried out to predict the process efficiency and subsequent potential biogas, regardless of the size and/or the operation mode (batch or continuous). The simulation showed the ability to overcome the uncertainty and discrepancy of measured biogas from an industrial digester. In the case of the lagoon digester, it was shown that the discrepancy in the measured biogas is around 250%. The measured biogas was higher by 2.5-fold than that predicted by simulation. In support of this, the theoretical biogas production from the anaerobic lagoon closely approximates the value obtained using BioWin simulation. The software was first calibrated with reliable measured data. Furthermore, different techniques were used to validate the agreement between the measured and predicted data, such as *R*-squared, *r*, *p*-value and the Willmott index of agreement, which all illustrated good agreement.

Altering the default parameters in BioWin in order to match its prediction with reliable measured data as a calibration procedure is a useful method for accurately predicting other unmeasured parameters. Furthermore, it provides information about the efficiency of the digester. The COD outlet from the anaerobic lagoon was successfully predicted over a long period of monitored data, around seven months, with less than 15% MAPE. Furthermore, the quality of the wastewater in the batch digester, in regards to COD content, was matched with that predicted by BioWin, with a MAPE around 7%. This was done using the measured hydrolysis rate (kinetic parameter).

It is obvious that solving the problems associated with the anaerobic process may raise the investors' interest in covered anaerobic digesters and, as a consequence, will remarkably reduce the emission of GHGs. The simulation of such a process could reveal the potential risks and associated costs that are not caught in capacity planning.

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Author Contributions

Both Ihsan Hamawand (first and corresponding author) and Craig Bailie (co-author) have made substantial intellectual contributions to the scientific investigation in this article. All authors have met the authorship criteria; Ihsan Hamawand has contributed significantly to the conception, design, execution, analysis and interpretation of the data; participate in drafting, reviewing, and revising the manuscript for intellectual content; and approve the manuscript to be published. Craig Baillie has contributed significantly to the conception, analysis and interpretation of the data; participate in reviewing and revising the manuscript for intellectual content; and approve the manuscript to be published.

Nomenclature

BMP	Biochemical methane potential
R-squared	Coefficient of determination
r	Correlation coefficient
p	Probability
SD	Standard deviation
CSG	Coal seam gas
BOD	Biological oxygen demands
GHGs	Greenhouse gases
COD	Chemical oxygen demand
FOG	Fat, oil and grease
AD	Anaerobic digestion
ASDM	Activated sludge/anaerobic digestion models
IWA	International Water Association
WWTP	Wastewater treatment plants
TSS	Total suspended solids
TKN	Total Kjeldahl nitrogen
NH_4-N	Ammonium nitrogen
NO_3-N	Nitrate
TP	Total phosphorus

PO_4-P	Orthophosphate
VSS	Volatile suspended solids
MAPE	Mean absolute percentage error $\text{MAPE} = \frac{100}{N} \times \sum_{i=1}^{N} \left\lvert \frac{x_i - \hat{x}_i}{x_i} \right\rvert$ where $\{x_i\}$ is the actual observation time series, $\{\hat{x}_i\}$ is the estimated or forecasted time series, and N is the number of data points
CSTR	Continuous stirred tank reactors
SRT	Solid retention time
HRT	Hydraulic retention time
DAF	Diffuse air flotation
MLA	Meat Livestock Australia
ISS	Inorganic suspended solids
VFA	Volatile fatty acid
TA	Total alkalinity
EGSB	Expanded granular sludge bed
DO	Dissolved oxygen
Fus	Unbiodegradable soluble gm COD/gm of total COD
Fbs	Readily biodegradable (including acetate) gm COD/gm of total COD
Fup	Unbiodegradable particle gm COD/gm of total COD
Fxp	Non-colloidal slowly biodegradable gm COD/gm of slowly degradable COD
Fac	Acetate gm COD/gm of readily biodegradable COD

Conflicts of Interest

The authors declare no conflict of interest.

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