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Simulation and optimization methods for maximizing biogas production in an anaerobic digestion process

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Abstract

Previous studies on the simulation and optimization of anaerobic digestion have mainly focused on experimental works. However, a review where these studies are synthesized into a cohesive summary published in a single paper is imperative. The review aims to provide recent ways of simulating and optimizing anaerobic digesters, thereby maximizing their biogas yield with the use of software tools. It addresses and provides an overview of the description and development of the process model, optimization techniques associated with biomass feedstock, mathematical model, and standard software used for process simulation. From the review, it is established that methane and carbon dioxide are the critical factors in determining the best optimum substrate ratio in an anaerobic digester. Also, the simulation of anaerobic co-digestion from the study is known to have a higher biogas yield than mono-digestion. The review reported that the stoichiometric method via path degradation is one way of building process simulation. Findings from the review reveal that the significant key optimization parameters are the predictors used for the development of the model, which are usually factors that affect anaerobic digestion. Hence, Aspen Plus, SuperPro Designer, and Response Surface Methodology are regarded as the most effective simulation software tools and optimization techniques employed for anaerobic digestion, respectively. This review article concludes by providing valuable insight into the recommendations, limitations of the study, and suggestions for future studies.

Keywords: Biogas yield, Co-digestion, Feedstock, Mathematical model, Software.

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1. Introduction

The conversion of organic waste to energy and biofertilizer is called anaerobic digestion technology. Several factors are responsible for the performance of anaerobic digestion, such as temperature, hydraulic retention time, pH, mixing, organic loading rate, etc. This is necessary to optimize the system's co-digestion (simultaneous anaerobic digestion of multiple organic wastes in one digester) for higher methane yield [1]. Hence, predicting dynamic behavior helps industries implement a real-time solution and make the best decisions, especially in industries. This is one of the essences of the simulation and optimization processes. Khanal, et al. [2] mentioned that process stability and optimization of anaerobic digesters can be achieved through models and simulation (process control strategies). Anaerobic digestion models are deficient in describing the process parameters when dealing with a transient state resulting from input changes. The recent mathematical model in the description of anaerobic digestion deals with a steady-state condition, where time series prediction is scarce in the literature. These models are considered deficient in illustrating the process parameters under start-up operation or transient conditions resulting from changes in input. According to Weinrich and Nelles [3], the dynamic model provides efficient and reliable operation for future digesters with a combination of available data and laboratory analyses.

The first dynamic model of the anaerobic digestion process was published in 1971 by Andrew et al., with unionized acid as a rate-limiting step. Three years later, Hill and Barth [4] developed a model that inhibits fatty acids in manure and animal wastes. Dynamic modeling of a batch biogas digester fed with cow dung was developed by Keshtkar, et al. [5] under mesophilic temperature conditions. Batstone, et al. [6] stated that anaerobic digestion model no. 1 (ADM1) is popular and widely accepted, with 12 algebraic and 19 differential equations and 24 dynamic variables. The application of models (mathematical and simulation) with respect to factors affecting anaerobic digestion enables the co-digestion anaerobic system to optimize and maximize methane production. With that in mind, research ought to be conducted to investigate and determine which process simulation model has the tendency to enhance the performance of anaerobic digestion, mostly on-demand bioenergy production. According to Inayat, et al. [7], the lack of information in the present model, as mentioned earlier, is recognized. However, developing new models may result in the build-up of the knowledge gap. Notably, the optimizing variables for anaerobic digestion are important for the performance of the process and identifying energy efficiency and cost-effectiveness. Process simulation and optimization often aim to design and describe a system to better understand operating and optimal working conditions. Also, its application extends to the control and forecast of the behavior and outcome of the anaerobic digestion system [8]. Due to this advantage, several researchers have employed this tool to guarantee efficient control and optimization of biogas production, thereby aiming to improve the system's performance. Mechanistic and data-driven (empirical) models are the classifications of anaerobic digestion models.

Mechanistic models focus on biological, physical, and chemical laws, while data-driven models deal with mathematical equations to determine the correlation between input and output parameters using measured and experimental data [9]. Models that use a defined set of differential equations to describe the laws of processes (biological and physicochemical) are also considered mechanistic models [10]. They comprise kinetic, ADM1, and stoichiometry models. This is because they are based on the growth of microorganisms, substrate conversion, and production of by-products. Hence, this model mostly considers the effect of pH, temperature, and inhibitory compounds on the system [11]. The main objective of the mechanistic model is to characterize the growth and inhibition of bacteria based on the substrate. Walid, et al. [8] listed the procedures for developing such a model; these include the interaction of the knowledge present between variables, the determination of the model parameters using the experimental data, and finally, the collection of data from the process (needed for validation) [12]. However, the International Water Association (IWA) developed a generalized model for the best simulation, known as the ADM1, an example of a mechanistic model. In this case, multiple steps were involved in describing the physicochemical reaction of ADM1, such as the dissociation and association of ions and gas-liquid transfer [6]. An example of the ADM1 for process simulation of the anaerobic digestion process has been widely explored in methane production. Hence, it is regarded as one of the most comprehensive anaerobic models available [13].

The data-driven (empirical) model is based on observations, data records, or measurements (response surface methodology, artificial neural network, and statistical models) [9, 14]. Its objective deals with patterning the behavior of the system in the absence of any prior knowledge of the occurring operations. The model combines and interacts with various disciplines, including mathematical modeling, statistics, information theory, and data science. Liakos, et al. [15] stated that the data-driven model is useful for identifying the structure of a given process together with correlation analysis of components without prior knowledge. In so doing, the learning process and the construction of knowledge need datasets or historical data. From the training phase, as a result of experience gained, the testing phase suffices immediately, after which models are focused by classification, prediction, or clustering referring to test data. Therefore, the analysis of the model is calculated via the performance measure, which enhances data training [15].

A more detailed discussion of the mechanistic and empirical models is presented in the methodology section under the optimization techniques of the anaerobic digestion process. In addition to that, the description and development of the process model and software used for process simulation were provided, including their respective process flow diagram. The result and discussion section presents recent studies and their findings related to the simulation and optimization of anaerobic digestion as a separate study and a combination of process simulation and optimization studies in a single study. Previous studies on the process simulation and optimization of anaerobic digestion have been based on experimental works, as seen in Inayat, et al. [7]; Tiong, et al. [16]; Qdais, et al. [17]; Nurgaliev, et al. [18]; Budhraja [19]; Ganeshan and Rajendran [20]; Kelif Ibro, et al. [21] and Menacho, et al. [22], etc. However, to the authors' best knowledge, reviews in which summaries of these studies' findings, objectives, and a lot more are limited in the literature. Therefore, the review aims to provide ways of predicting the performance of an anaerobic digester, thereby enhancing its biogas yield by applying mathematical and simulation models from the literature and determining the most effective optimization technique for biogas production. To achieve this aim, the following objectives will be established.

1. To determine the description and development of the process model for anaerobic digestion.
2. To investigate the software used for process simulation and optimization techniques.
3. To evaluate the techniques or approaches for the optimization of anaerobic digestion.
4. To review studies in connection with the simulation and optimization of anaerobic digestion.
5. To provide recommendations where necessary and identify areas of future studies in relation to the topic.

2. Methodology

2.1. Description and Development of the Anaerobic Digestion Process Model

Model description and development aimed at forecasting the dynamic behavior and performance of the anaerobic digestion process. Most process simulation and optimization models use a set of differential equations to characterize different stages of anaerobic digestion, such as hydrolysis, acidogenesis, acetogenesis, and methanogenesis [20]. Figure 1 shows the different stages of the anaerobic digestion process. However, acid and methane formers are responsible for the microbial communities present during the various stages of anaerobic digestion, as shown in Figure 1.

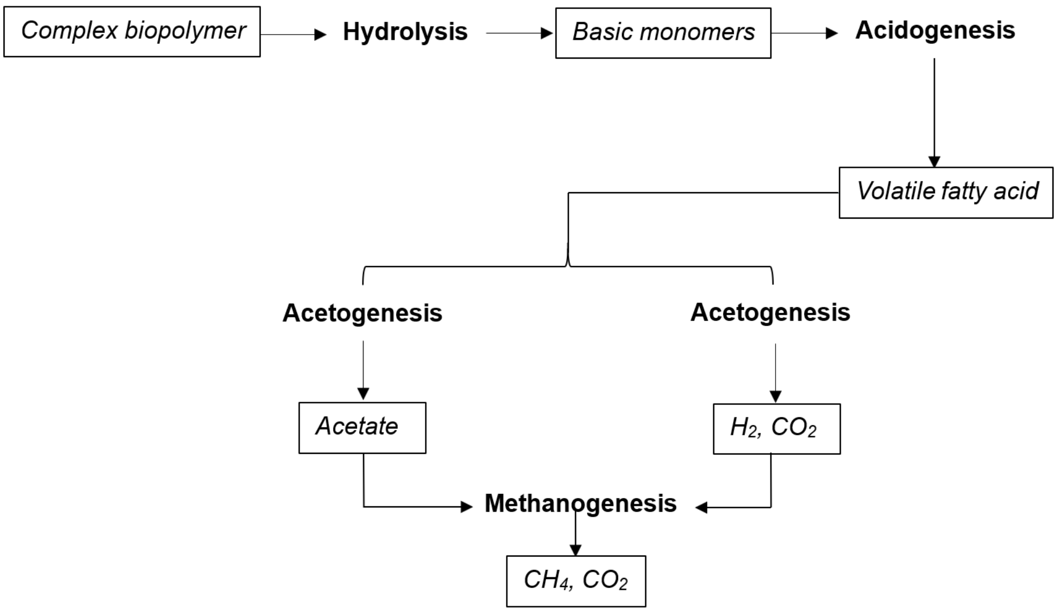

Figure 1.
Stages of the anaerobic digestion process.
Source: Uddin and Wright [23]

During the development of a model for process simulation and optimization, the key input parameters (predictors) are the factors that affect the performance of the anaerobic digester, and the output variable is the biogas yield, while the monitoring parameter (for instance, death rate and kinetic co-efficient) takes place or is considered in the model as shown in Figure 2.

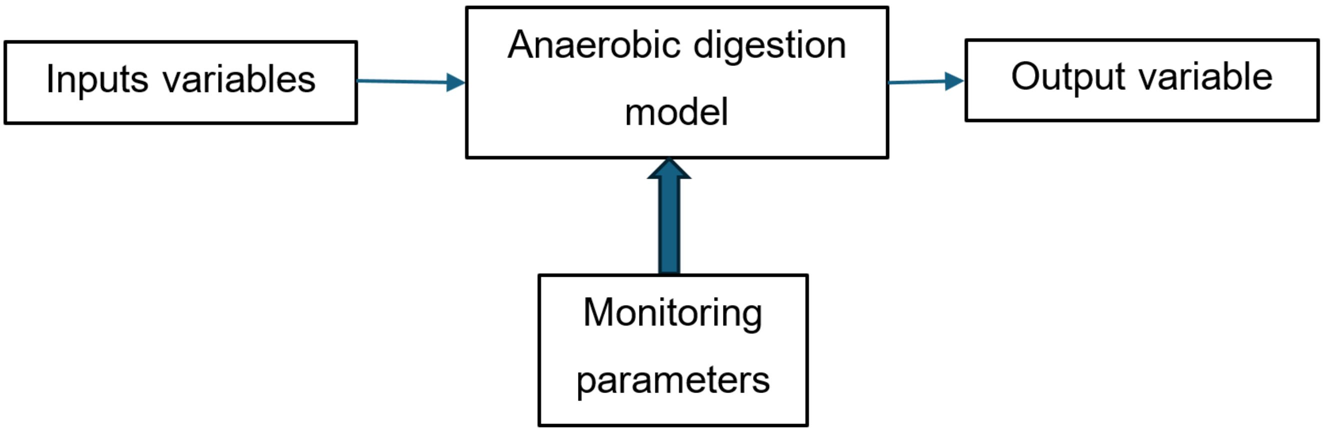

Figure 2.
Simple block diagram describing the development of the process model.
Source: Ganeshan and Rajendran [20].

Most of the model development from literature are equations describing and illustrating the hydrolysis and acidogenesis stages involved in anaerobic digestion. A study conducted by Ganeshan and Rajendran [20] mentioned these equations. According to Ganeshan and Rajendran [20], various scenarios are present during the development of process simulation and optimization models. For instance, in the case of a change in volatile solids concentration in the digester during the digestion process, a change of volatile solids concentration in the digester lading rate with kinetic as well as rate of change in total volatile fatty acid obtained by adding volatile fatty acid produced with the difference between the growth rate of the acid and methanogens formers. These cases are known to take place or occur during the hydrolysis and acidogenesis stages.

2.2. Software used for Process Simulation and Optimization of Anaerobic Digester

Anaerobic digestion can be carried out using software for simulation and optimization purposes. This software is designed specifically for modeling anaerobic digestion processes, overall process simulation and optimization, and different operational parameters in the anaerobic digestion process. Inayat, et al. [7] mentioned that standard software used for process simulation and optimization includes Aspen Plus, SuperPro Designer, BioWin, Computational Fluid Dynamics (CFD), and MATLAB.

2.2.1. Aspen Plus (AP)

Aspen Plus is software used for chemical process simulation, which allows and enables the simulation of a process model and design and enhances existing designs using complex equations. One major advantage of Aspen Plus is that it simulates the actual behavior of the digester by using the fundamental engineering relationships of mass and energy balances and phase and chemical equilibrium [24]. Through Aspen Plus, many industrial modules are built using different process flow sheets conducted and simulated by interconnecting modules. Aspen Plus is considered the simplest software for any parametric study of anaerobic digesters. This is attributed to its efficiency, with modules that depend on complexity and precision. Inayat, et al. [7] recommend Aspen Plus as the most effective and simplest method to simulate an anaerobic digester due to its efficient results. Hence, the limitation of using Aspen Plus deals with its high cost for process design, which often does not cover a specific type of simulation, and the complexity of model development (time-consuming and requires detailed knowledge of thermodynamics and chemical kinetics) for computational efforts. In addition, several assumptions are required while using Aspen Plus in the development of the model.

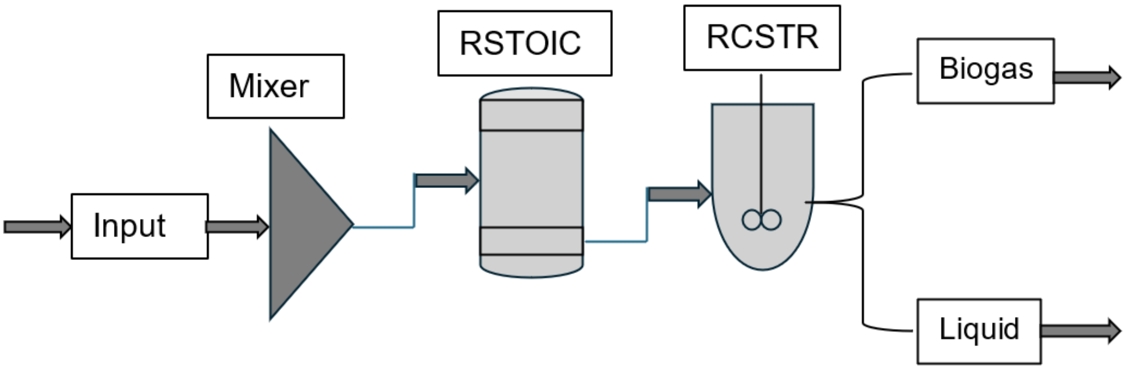

Figure 3.
illustration of Aspen Plus for a simulation model of anaerobic digestion.

2.2.2. Super Pro Designer Software

The SuperPro Designer is useful for modeling, evaluating, and optimizing integrated processes, especially in various industries. These industries include pharmaceuticals, Biotech, specialty chemicals, food, consumer goods, mineral processing, microelectronics, water purification, wastewater treatment, and air pollution control. Mokraoui, et al. [25] conducted a study where SuperPro Designer Software was used to model and simulate biomass anaerobic digestion for optimum biogas yield and carbon dioxide mineralization. The software can be used at all stages of the process development, from conceptual design to process operation, simulation, and optimization. Besides the process simulation and optimization, SuperPro Designer calculates mate-rial and energy balances, equipment sizing and costing, process economics, and waste stream characterization [26]. The software's limitation deals with its default values for many input data required for simulation. Hence, it has less rigorous thermodynamic packages. Some streams during continuous processes must be known beforehand [27]. Figure 4 shows the SuperPro De-signer Software version 8.5 by Intelligent Inc. used in Mokraoui, et al. [25] study for modeling and simulating biomass (municipal waste, date seed/leaves, and food waste) anaerobic digestion. Recall that the major composition of biomass is carbohydrates, proteins, and fat.

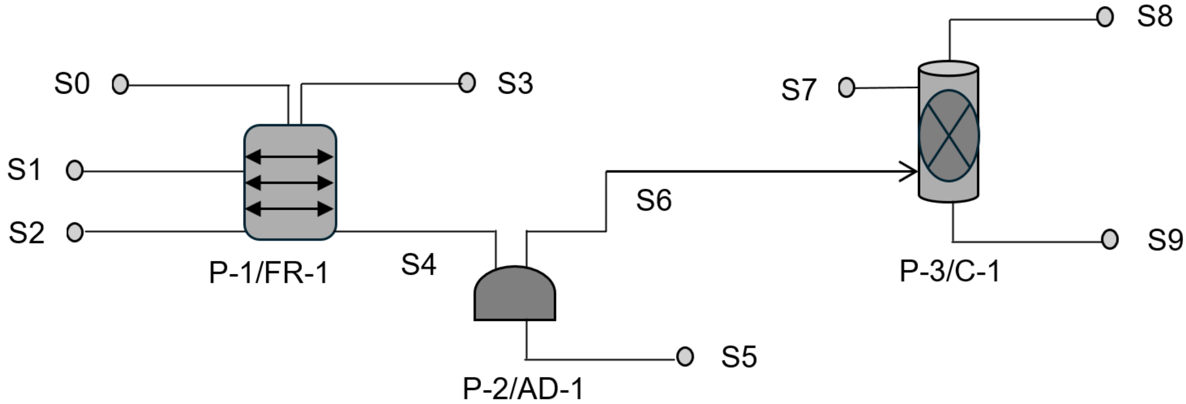

Figure 4.
Super Pro Designer for simulation of anaerobic digestion.
Source: Mokraoui, et al. [25].

The description of the processes used in Figure 4 is defined in Table 1.

Table 1.
Definition of processes in Figure 4.

Processes	Definitions
S0	Water
S1	Media
S2	Air
S3	Vent
S4	Broth
S5	Digestate
S6	Crude biogas
S7	MgO/H_20 (inlet stream)
S8	Sweetened biogas (outlet stream)
S9	$MgCO_3$
P-1/FR-1	Fermentation reactor
P-2/AD-1	Digester reactor
P-3/C-1	Absorption column

Figure 4 shows that three stages of reactions are employed. These include the fermentation unit (P-1/FR-1), the digester unit or reactor (P-2/AD-1), and the absorption column (P-3/AC-1). The P-1/FR-1 involves the fermentation kinetic, where the hydrolysis reaction occurs, usually under batch process. P-2/AD-1 uses a stoichiometry reaction to produce biogas in an anaerobic digester at 37°C (mesophilic temperature) and 1 atm. It also represents the degradation of amino acid, acetogenesis, acidogenesis, and methanogenesis. Two streams (S6 and S5) are dis-charged from the digester reactor. Similarly, the absorption column contains the inlet and outlet stream (S7 and S8), respectively, and was set at a temperature of 200°C. Interestingly, the SuperPro Designer is also used for calculating mass and energy Mokraoui, et al. [25].

2.2.3. MATLAB and Simulink

MATLAB/Simulink are known as software programs capable of simulating anaerobic digestion and wastewater treatment system control [28]. This was revealed in a study conducted by Saeed, et al. [29] as shown in Figure 3. The study simulated a biogas power reactor with animal manure under different operating conditions to achieve a 70 – 75% methane concentration. The authors recommended the MATLAB/Simulink model as effective and robust, focusing on the differential equation of 4 stages of anaerobic digestion. During the literature review, this area of the study model by Saeed, et al. [29] is limited. MATLAB/Simulink is useful in optimizing production performance, minimizing operating costs and downtime, and maximizing return on investment. With the application of MATLAB/Simulink, design, modeling, and simulation of dynamic, multi-physics systems at the component, equipment, production line, or asset level is possible. Also, it speeds up big data analysis with computer vision, data science learning, and deep learning, including high-power computing capabilities. Figure 5 shows the Simulink model for biogas digester through MATLAB.

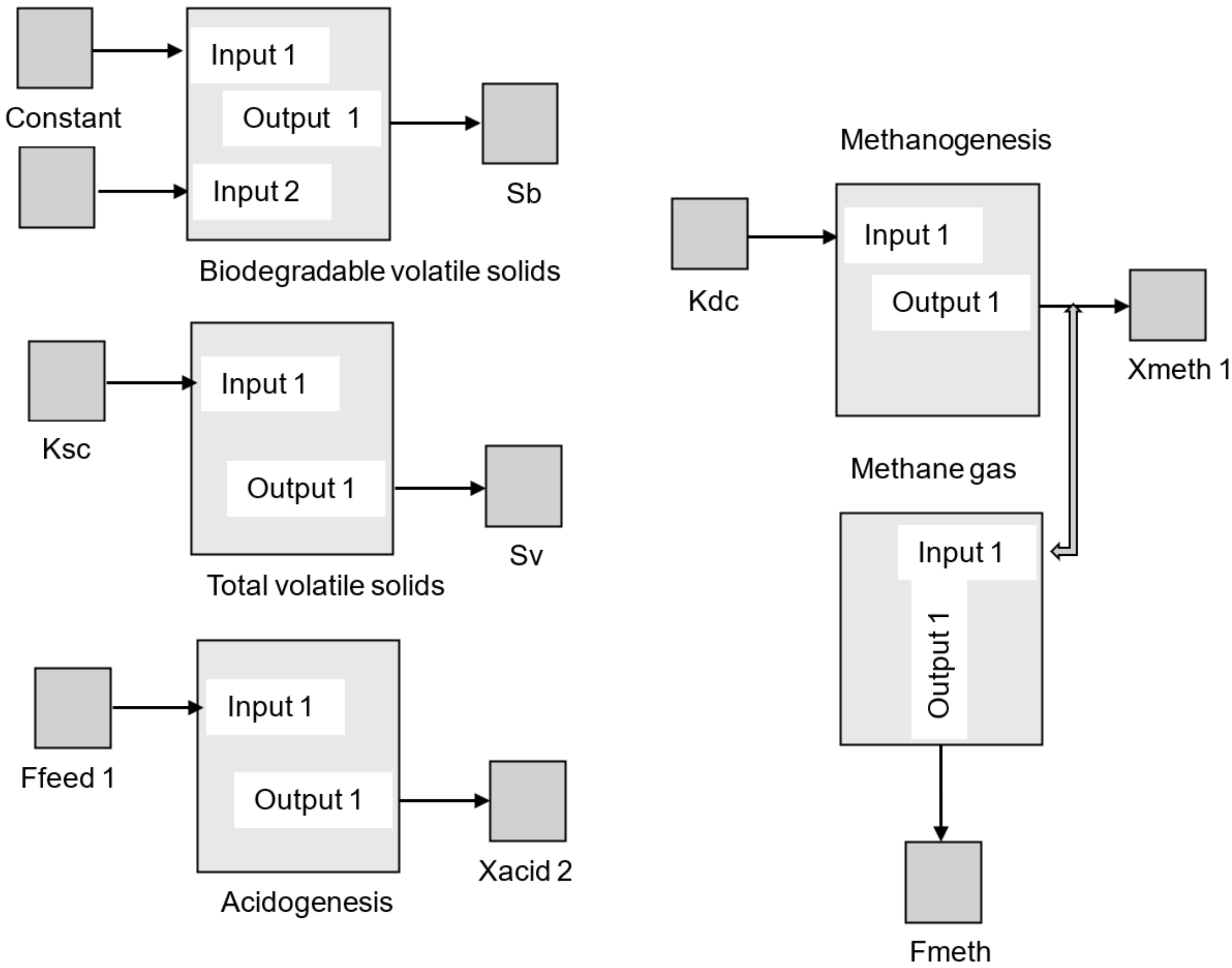

Figure 5.
Simulation model using Simulink via MATLAB.

Table 2.
Definition of abbreviation used in Figure 3.

Abbreviation	Definitions
Xmeth	Concentration of methane (kg/m^3)
Xacid	Concentration of acid (kg/m^3)
Sv	Concentration of total solids volatile fatty acid (kg/m^3)
Sb	Concentration of biodegradable volatile solids (kg/m^3)
Ksc	Monod half velocity constant for methanogens (kg/m^3)
Ffeed	Feed flow rate (m^3/day)
Kdc	Specific death rate of methanogens (d^{-1})

2.2.4. Bio Win Simulator

The simulation of the anaerobic digestion process can be carried out using BioWin software. It is a window-based computer simulation model developed by EnviroSim Association Ltd. The software is easy to use but requires extensive knowledge and experience in wastewater treatment processes [30, 31]. Notably, BioWin has been known as an excellent tool for designing and analyzing wastewater treatment plants (WWTP). The software has also found its way into the chemical oxygen demand (COD) removal simulation and the subsequent biogas generation rate. For instance, it was found in two abattoirs, as reported in Hamawand and Baillie [28]. In this case, the accumulation of crust (high content of fat, oil, and grease) seems to be an issue [28]. The simulator can configure the various sludge reactor dimensions, as mentioned by Oleszkiewicz, et al. [32]. With BioWin, it is possible to predict the rate of biogas production and the quality of wastewater ponds. Usually, this is impossible because of the high accumulation of crust and damage to the pond's cover. However, using the software provides a preliminary assessment of the pond's performance and the biogas production rate. Furthermore, it simulates both small- and large-scale biogas digesters with a mean absolute percentage error of less than 10%, and the index values are good. It requires a large amount of data for an accurate model prediction. If not, the model prediction is inaccurate and unresponsive to varying operating and environmental conditions. In addition, in-depth data collection and analysis are required for further development and refinement of the models for emissions. Figure 6 shows a schematic of food waste for anaerobic digestion using BioWin.

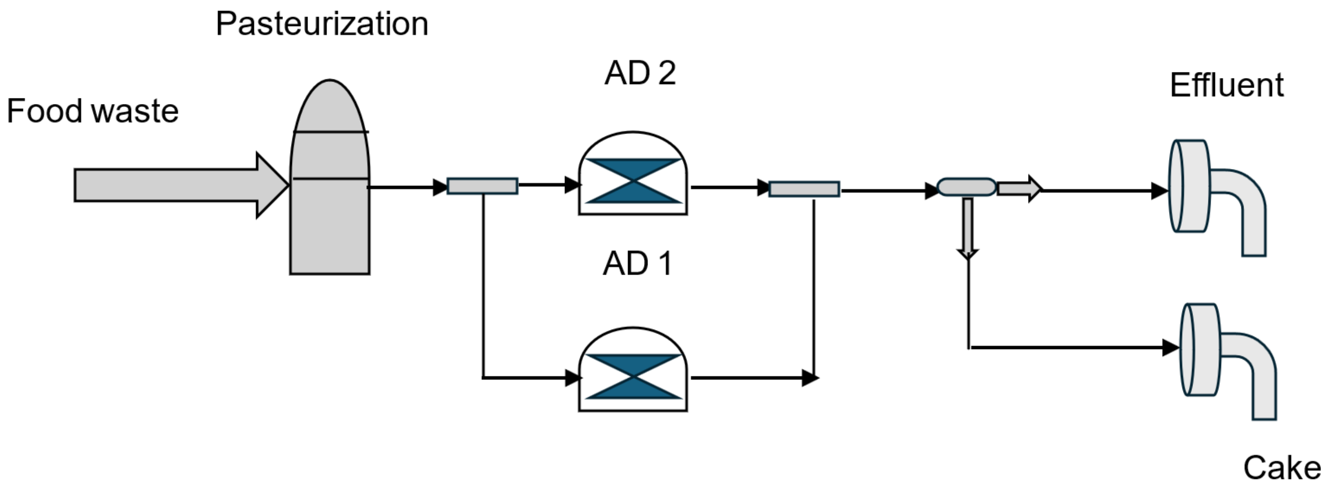

Figure 6.
Flow diagram illustrating anaerobic digestion of food waste used by BioWin.
SOURCE: Forgacs, et al. [33].

2.2.5. Worldwide Engine for Simulation Training and Automation (WEST)

WEST is known as friendly simulation software and has been developed and updated with drag-and-drop interfaces. This allows for easy assembly and digester configuration, facilitating the use either by basic knowledge or no expertise as a modeler [34]. Moreover, simulators, like the WEST, provide better decisions and have an environmental and economic impact. According to WEST Vangheluwe and Claeys [35] the software provides a platform for existing models to implement and test new ex-tended models and can be described as a structured collection of differential-algebraic equations (DAEs) for the activated sludge (AS) process [36, 37]. Interestingly, the software has an extensive model library, including the different models for activated sludge units, fermentation, and settling tanks. Simulators such as WEST came about to address the constraint associated with academic research and real knowledge as well as capabilities of wastewater and anaerobic digester professionals, which gives the right to incorrect application of the model, thereby promoting the negative perception of simulation tools [34]. DHI Denmark develops the WEST soft-ware, which is known to be flexible and provides an interactive platform to simulate anaerobic technologies. The WEST simulator, this is divided into 4 elements, as shown in Figure 7.

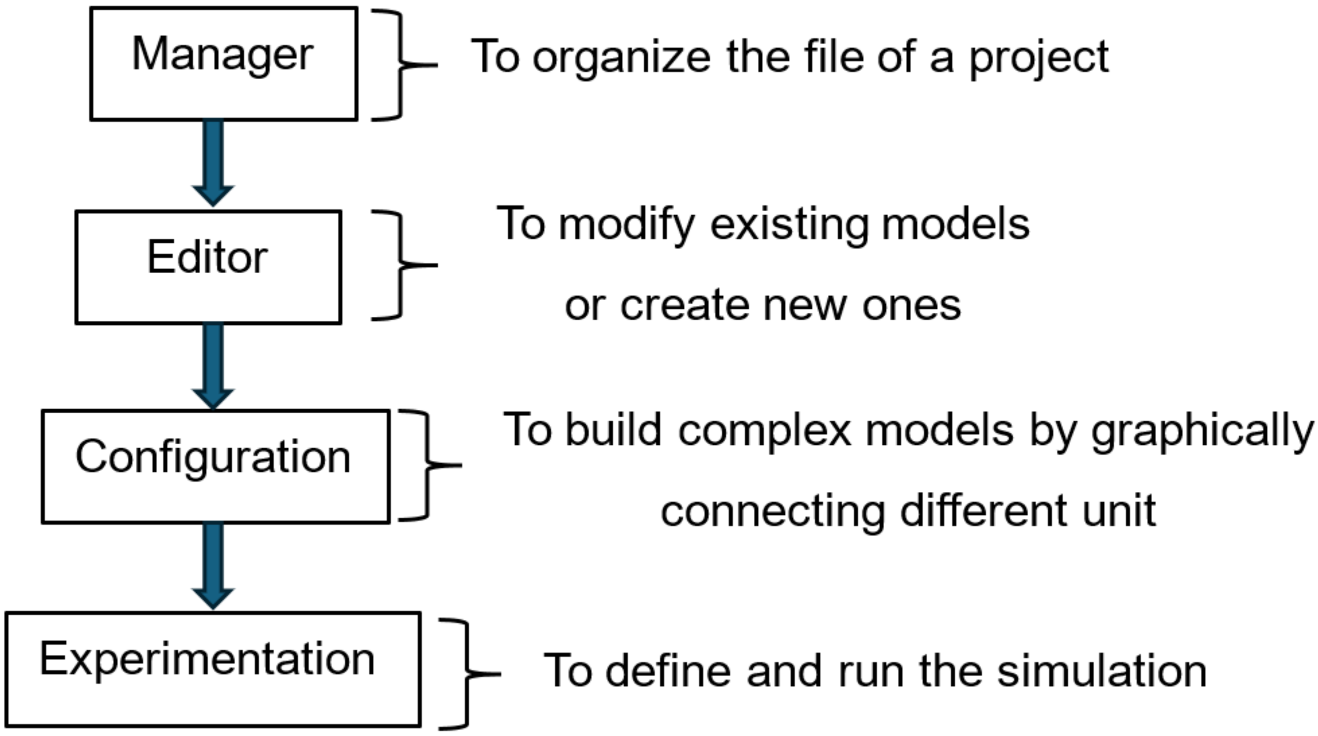

Figure 7.
Elements of the WEST simulator.

These elements in Figure 7 aim to facilitate and optimize the implementation and reuse of knowledge associated with the treatment of wastewater models. With the WEST modeling and simulation environment, a strict distinction is possible between the modeling environment (aim to enable reuse of model knowledge) and the experimentation environment (focusing on maximizing accuracy and performance) [37].

2.2.6. Sewage Treatment Operation Analysis over Time (STOAT)

The Water Research Centre (WRC) developed the software package in 1989 as computer-based, integrating a dynamic wastewater treatment process model into a series of research projects. simulating its processes [38]. The essence is establishing better planning and operational procedures and gaining significant cost-effectiveness. It is worth mentioning that STOAT software is a free modeling package for numerical modeling and simulation of digesters and reactors, mostly for wastewater treatment. For this purpose, the software evaluates the effects of in-fluent physiochemical properties and water flow rate on pollutant removal efficiency. However, the software is useful and said to be a reliable tool for predicting and optimizing oxidation ditch processes Huang, et al. [39]. Abdulla and Farahat's [40] study reported that the software could model activated sludge systems, bio-film-based processes, and treatment. Moreover, its application has been widely used globally because of its capability to achieve relatively simple data requirements and free availability as a dynamic sewage treatment works modeling. Issa Abdulla and Farahat [40] reported that previous studies mentioned that STOAT had been used to optimize the design possibilities of modifying and renovating abandoned plants or reactors. Hence, this is considered the potential of dynamic simulators in optimizing and developing the design of reactors or plants. Figure 8 shows the STOAT process flow diagram.

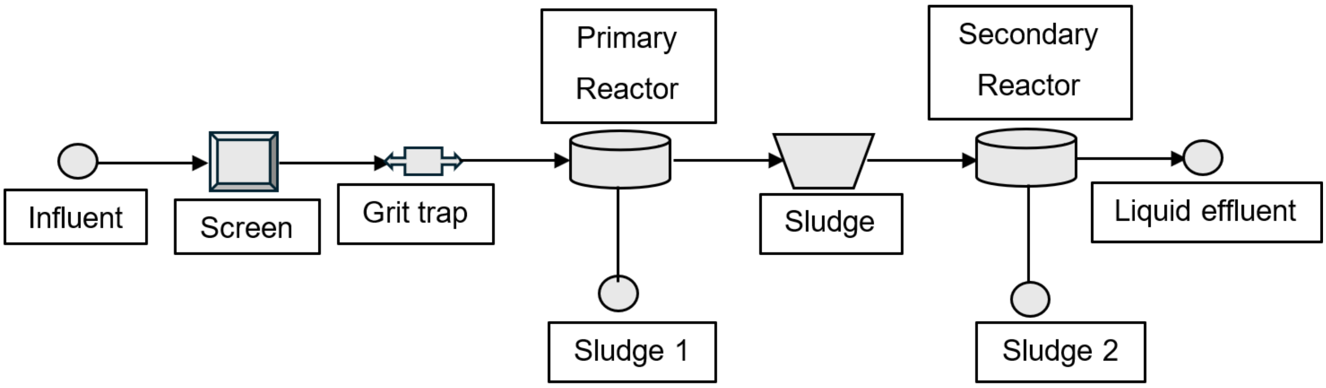

Figure 8.
Process flow diagram of Sewage Treatment Analysis over Time.

2.2.7. ChemCAD

ChemCAD is referred to as an integrated suite of intuitive chemical process simulation software that fits into the chemical engineering workflow, thereby supercharging the efficiency of an engineer. It is designed to model, simulate, and optimize chemical processes. ChemCAD has numerous applications, including performing thermodynamic calculations, creating heat and mass balances, designing and analyzing equipment, simulating dynamic behavior, optimizing plant operations, and making informed decisions in oil and gas, pharmaceuticals, chemicals, and renewable energy [MathWorks- https://nl.mathworks.com > connections > product_detail]. The adsorption process was optimized by simulation using ChemCAD simulation software. The essence was to purify biogas through water scrubbing based on an absorption process using pressurized water as a solvent, as studied by Sugiharto and Hidayat [41]. Using ChemCAD, two factors are responsible for its simulation results. These include the thermodynamic model and calculation model. The thermodynamic model via Wilson simulates vapor–liquid equilibrium (VLE), whereas the calculation model is based on a rigorous calculation method [41]. In a similar study, the process simulation of methane's cleaning and enrichment process was conducted using ChemCAD (steady state process from Chemstation). During the simulation process via ChemCAD, Masebinu, et al. [42] reported that the dynamic and unsteady state process PSA unit was represented with a component separator unit operation. This was constrained to the digester, thereby resulting in the removal of H2O and H2S. From the simulation result, the cleaning process effectively eliminated vapor and the content of H2S in the biogas, whereas nitrogen was reduced to an acceptable limit [42]. Another case study of the application of ChemCAD was seen in Gawel [43] study. The study used ChemCAD simulation software for the performance characteristics, design, optimization, and absorption costs used to purify biogas in a digester. With ChemCAD, the mixtures for agricultural biogas were purified below 1% volume of CO2 and 4 x 10^-4% mass of H2S. These mixtures were entered into absorption and desorption units, and simulations were provided. The simulation result revealed that the design parameter was calculated and entered into each unit, as well as the cost estimation section, to estimate the purchase costs of the apparatuses. The calculation found that the absorbent mixture allows biogas production at the lowest estimated cost for ten years.

Having looked at the various software packages used for process simulation and optimization; Table 3 presents an overview of these software tools.

Table 3.
Summary of various software tools used in the study.

Aspen Plus	SuperPro Designer	Matlab/Simulink	BioWin	WEST	STOAT	CHEMCAD
The software is capable of simulating chemical reactions in petroleum and chemical processes.	It facilitates modeling, evaluation, and optimization of integrated batch and continuous processes.	It has outstanding features of a series of mathematical functions and is an easy-to-learn language.	The simulator is used worldwide to analyze and design wastewater treatment plants.	It is one of the most complete, user-friendly, and widely used systems in wastewater treatment. Hence, users can implement their own models.	The package contains integrated dynamic models of the processes used in wastewater treatment.	The software is applicable for a wide range of use cases in chemical processing projects.
It has the ability to develop both steady-state and dynamic models of the anaerobic digestion process.	Used as a valuable tool for addressing environmental issues such as wastewater and air pollution.	Capable of developing a simulation flow model for anaerobic digestion.	The software runs two types of simulators (steady state and dynamic).	The software is divided into four (manager, editor, configuration, and experimentation).	It has a computational speed that permits rapid investigation of a range of sewage systems.	Handle small and large problems simultaneously and a wide range of use cases in chemical projects.
It predicts the behavior of the anaerobic digestion processes.	Analyzes the effect of changes in operating conditions on the process economy.	It is a good start for the development of complex concepts for the optimization sector coupling.	The software is built upon the activated sludge model and anaerobic digestion mode.	The software provides a flexible and interactive platform for the simulation of different wastewater treatment plants.	Applicable for process optimization and design, as well as the feasibility of dynamic modeling.	Consists of a large system database of standard components and a vast thermodynamic library.
The software provides the specifications of the desired kinetic model that can handle multiple reactions simultaneously.	Flowsheet-driven simulator software for material and energy balances, sizing and costing equipment, economic evaluation, environmental impact assessment, and process scheduling of batch and continuous processes.	The software, in terms of the graphical interface, facilitates the design of a block-based simulator. This makes it easier to visualize and adjust parameters for various stages of anaerobic digestion.	It provides a plant modeling process that gives insight regarding cost reduction, capital costs, and operating expenses.	The activated sludge models (ASM) developed by the International Water Association (IWA) and other models describing biological carbon and nutrient removal processes are implemented only in the WEST simulator.	Used to investigate the feasibility of dynamic modeling of an entire wastewater treatment plant using the simulation of individual unit processes.	State-of-the-art process simulators used in the engineering community, for instance, as a process optimization tool.

Source: Hussain, et al. [44]**;** Pal, et al. [45]**;** Senthilkumar and Yuvaperiyasamy [46]; Callahan, et al. [47]; Ruiz, et al. [34] and Abdissa Akuma, et al. [38]

Table 4.
The Modeling techniques for the anaerobic digestion model.

Mechanistic model		
Types	Notes	References
Kinetic model	This is used to express the conversion of substrate rates in anaerobic digestion systems. Examples of such models include the first-order kinetic model, Monod, and the modified Gompertz model.	Xie, et al. [48]
ADM1	The ADM1 is a complex mathematical model used to describe the physical and biochemical processes of anaerobic digestion systems. The model contains up to 86 parameters, applicable to a range of substrates such as industrial, municipal, and domestic wastewater, as well as agricultural waste under various operating conditions. Hence, the results of the ADM1 are known to be expressed in terms of chemical oxygen demand (COD).	Ramachandran, et al. [49]; [50] and García-Diéguez, et al. [51]
Stoichiometric model	Here, the model deals with the equilibrium constant from the chemical reaction to predict the amount of CH4 and CO2 generated from a particular substrate. For the stoichiometric model, three factors are responsible for the handling of the biomass. These include the presence of dry waste in the reaction, moisture content, and the conversion of dry waste into ash. Using the stoichiometric model, the Buswell formula is an example of an equation used to predict biogas yield.	Silva, et al. [52]
Empirical (data driven) model		
Computational fluid dynamic (CFD)	This is mostly used to develop a model capable of predicting the hydrodynamic behavior of the liquid stream in the digester. It is affected by agitation, dispersion, diffusion, convection, the external environment, and limiting conditions. With the application of CFD simulation, it is used to select and optimize the best impeller and its conditions for the agitation process. However, the speed of agitation usually influences biogas production. Using CFD simulation helps to model the velocity flow inside the digester.	Dabiri, et al. [53] and Pukkella, et al. [54]
Artificial neural network (ANN)	An artificial intelligence method that mimics the human brain to predict the performance of linear and non-linear processes. It operates under different layers such as the input, output, and hidden layers. In the ANN algorithm, the dependent and independent variables are connected to the neuron for the purpose of saving and using the information to generate output data. Hence, modifications of the ANN exist, which include the feedforward neural network, backward propagation of errors, recurrent neural network, counter propagation, radial basis function network, and fuzzy-based algorithm.	Ramachandran, et al. [49] and Almomani [55]
Statistical models	Examples of such models include simple linear regression models, multiple linear regression models, fractional factorial designs, and systematic approaches. With reference to other models, the statistical models are simple and easier to understand with a monitored small number of explanatory variables.	Xu, et al. [56] and Ray, et al. [57]
Response surface methodology (RSM)	The RSM is a combination of the mathematical and statistical methods used for modeling, optimizing, and analyzing the effect of various parameters on a specific variable. Three steps of statistical design of experiments are involved in the RSM. These include the prediction of the coefficients in a mathematical model, estimation of the reaction, and suitability of the model.	Lin, et al. [58]

2.3. Techniques for Optimization of Anaerobic Digesters

Techniques for optimizing an anaerobic digester can be classified to focus on the mathematical aspect and the substrate. The mathematical aspect is regarded as modeling (involving equations), whereas the substrate deals with feedstock and inoculum, co-digestion, additives, and pre-treatment methods. Modeling provides solutions to the drawbacks of several techniques used to optimize anaerobic digesters. Modeling as an optimization technique helps to reduce the cost of investment, the requirement for energy, and the environmental load [11]. Anaerobic digestion models are employed to predict the behavior and outcome of an anaerobic digestion system and the optimal working conditions. Moreover, modeling for anaerobic digestion comprises mechanistic and empirical (data-driven) models. Table 4 presents the different types of modeling for optimizing an anaerobic digester.

3. Results and Discussion

3.1. Simulation of Anaerobic Digester

The simulation tool for the biogas digester is necessary to address the time-consuming and inaccurate aspects associated with the experimental procedure. In practical applications, the process simulation results are incorrect if inappropriate assumptions and software are not employed [7]. There have been limited studies dealing with the simulation of biogas digesters. However, ADM1 is a common and frequently used tool for simulating anaerobic digesters [59-61]. Interestingly, simulation studies have been conducted for olive mill wastewater, solid waste using ADM1, municipal solid waste organic fraction, and sewage sludge through the ADM1 modeling approach [62]. Simulation can be carried out to predict the efficiency of the anaerobic digestion process and potential biogas, irrespective of the size and mode of operation. The application of simulation is that it can overcome the uncertainty and discrepancy of measured biogas, especially from an industrial biogas digester [28].

In a study conducted by Inayat, et al. [7], Aspen Plus was used to simulate the performance of a biogas digester using wastewater and animal manure for biogas production. The Aspen Plus simulator was used in the study because it allows designing a simple biomass digester for multiple feeds without specifying the kinetic and specific reaction mechanisms. As part of the methodology of the study, it is imperative to point out that the composition of the inlet and outlet streams concerning the properties of biomass assists in building a simple anaerobic co-digestion. In the study, the author mentioned the mole fractions of CH_4/CO_2 as the critical factor for determining the best optimum substrate ratio. This was the basis of their simulation results, which contain the co-digestion of three cases (Case 1, 2, and 3) with date seed waste as biomass and date tree leaf and coffee water as biomass for cases 4 and 5, respectively. Case 1 includes 50% wastewater, 25% cattle manure, and 25% biomass; case 2 (34% wastewater, 33% cattle manure, and 33% biomass) and case 3 (50% wastewater, 35% cattle manure, and 15% biomass). The simulation results revealed that case 1 reported a gas stream of 47.85 mole % of CH_4 and 20.80 mole % of CO_2 for biogas production. Case 2 reported a gas stream of 46.30 mole % CH_4 and 29.65 mole % CO_2, whereas case 3 obtained a gas stream of 50.11 mole % CH_4 and 31.93 mole % CO_2. On the contrary, cases 4 and 5 obtained a gas stream of 50.55 mole % CH_4 and 31.56 mole % CO_2, as well as 47.13 mole % CH_4 and 31.95 mole % CO_2, respectively, for date tree leaf and coffee water as biomass. The simulation results showed that the optimum ratio of wastewater, cattle manure, and biomass in the slurry to maximize methane production was found in case 1, and the biomass feedstock is the date seed waste. This is because it has the highest CH_4/CO_2 ratio of 2.3. On the other hand, the study's best biomass for maximum methane production is the date tree leaves. This implies that simulation makes it possible to determine the optimum ratios of the substrate in slurry fed into the biogas digester for the anaerobic co-digestion process.

With the application of simulation using Aspen Plus software, it is possible to predict and evaluate the amount of biogas produced from co-digestion of cow dung and food waste. Evidently, this was shown in the study conducted by Nduse [24]. The authors employed the stoichiometry method to estimate the amount of biogas released from co-digestion, thereby calculating the electrical production potential. The study methodology involves the development of a three-case model using Aspen Plus. Case 1 and Case 2 deal with food waste and cow dung as single feedstock, respectively, and Case 3 is the co-digestion of both food waste and cow dung. The stoichiometry method was used to define various degradation reaction paths, such as glucose, galactose, xylose, sucrose, acetic acid, etc. According to the authors, the model for the process simulation was based on the degradation paths that produce CH_4 and CO_2 as end products. The obtained results for methane production from the simulation following the stoichiometry method were 0.726 kg/h, 2.496 kg/h, and 3.509 kg/h for Cases 1, 2, and 3, respectively. On the contrary, for the electrical potential, the values were 97.45 kWh, 285.26 kWh, and 401.02 kWh for Cases 1, 2, and 3, respectively. As seen in the previous study, in terms of the mole ratio of CH_4 and CO_2 (biogas composition), the mole fraction of the three cases for CH_4 are 0.05, 0.15, and 0.22, while that of CO_2 includes 0.05, 0.15, and 0.22. From the findings, it is revealed that path degradation shows equal moles of CH_4 and CO_2 produced in the stoichiometry reaction used in the simulation. This implies that the stoichiometry method through path degradation is one way in which process simulation can be built. The same applies to the Wukovits, et al. [63] study. From the study, it is established that higher biogas yield is realized through the simulation of anaerobic co-digestion than mono-digestion.

Simulation of anaerobic digestion requires complex mathematical models and optimization of numerous model parameters, as mentioned by Kovalovszki, et al. [64]. To establish this, Kovalovszki, et al. [64] conducted a study on the systematic methodology to extend the applicability of the bioconversion model for the simulation of various co-digestion scenarios. The authors used the BioModel software tool implemented in MATLAB combined with a Microsoft Excel-based data input and output platform to simulate a biogas digester using manure, wastewater, and organic substrate. Due to the presence of the manure used in the study, BioModel was utilized since it focuses on ammonia inhibition, which is relevant in manure-based digestion. Based on this, it involves a detailed description of pH and temperature to simulate free ammonia concentration. Furthermore, the software features a more convenient and mass-based unit system, which allows the characterization of substrates and products using simpler sampling and measurement techniques for slurries and solid waste. All these are said to be lacking in ADM1 when compared with BioModel software. The study aims to develop a parameter estimation methodology for improving anaerobic biogas digester modeling. To achieve this aim, the authors simulated anaerobic digestion via the MATLAB model in one anaerobic fermenter with the inoculum composition as the primary substrate and three optional co-substrates. The study methodology involves four steps, including the selection of parameters, analysis of sensitivity parameters, estimation of parameters, and evaluation. Biogas and methane production were the input parameters, whereas the volatile fatty acid, total ammonium, nitrogen-TAN concentration, and pH were chosen as the outlet parameters. Sensitivity analysis is used for the sampling-based Partial Rank Correlation Coefficient (PRCC) method. With BioModel software, identifying sensitive parameter complex bioconversion and estimating their value is possible. The authors' findings from the evaluation of the results show that simulation using general parameters fitted experimental data quite well, implying that it offers a reliable reference point for future simulation associated with anaerobic co-digestion.

Technological challenges are involved while dealing with anaerobic digestion. To address this, the study by Mokraoui, et al. [25] recommends computational process modeling and simulation, which provides realistic information. In their study, modeling and simulation of the simplified anaerobic digestion process were conducted using SuperPro Designer software with biomass feedstock containing carbohydrates, proteins, fats, and yeast. The study conducted the simulation of the pre-treatment of the substrate and anaerobic digester process using a stoichiometric fermentation reactor and an anaerobic digester reactor, respectively. This was carried out under a mesophilic temperature of 35°C, and municipal waste, date seeds or leaves, and food waste were used as substrates for digestion. 89.655% and 10.345% of CH4 and CO2 were obtained through the model simulation process of the anaerobic digester. The high percentage yield of CH4 was attributed to the carbohydrate feedstock, which produces a higher CH4 composition in biogas. The model simulation result confirms that the percentage of methane is always higher than carbon dioxide. From the result, the simulation of an anaerobic digester serves as a guide for realistic, scalable production as well as a strategy for refining biogas to produce a high amount of methane.

To develop a mathematical model for the batch study of anaerobic digestion of organic fractions of municipal solid waste (OFMSW), Manjusha and Beevi [65] adopt the default ADM1 for the modeling and simulation of anaerobic digestion and calibrate the model using lab-scale data. The study aims to use ADM1 to investigate the effect of different parameters used in the model on biogas production. Notably, ADM1 provides complete information about the physio-chemical reactions in the anaerobic process. These parameters for the development of the model include pH, volatile fatty acid (VFA), temperature, and retention time, which were implemented in MATLAB. Usually, ADM1 models are known to describe the five biochemical steps involved in an anaerobic digester (starting from integration followed by hydrolysis, acidogenesis, acetogenesis, and methanogenesis). According to the authors, 26 compounds are present in the ADM1 model, and biomass is recognized as an important component. Looking at the batch reactor model, Dittmer, et al. [66] implemented a differential equation using ADM1 to describe the 33 state variables via the Euler method solver ODE15s. The study results show that at initial low VFA accumulation, this increases at the end of the digestion due to the acidification of vegetable waste. This had a reduction effect on the pH and caused a decrease in the free ammonia and inhibition of the methanogenesis process. Furthermore, the performance of anaerobic digestion of solid waste showed maximum biogas production at a total concentration of 90 g/l. The concentration of biogas production was reduced due to a lack of substrate. On the other hand, increasing the concentration resulted in high production due to the accumulation of a large amount of substrate.

Due to the deficiency of reliable measurement technology and process monitoring associated with ADM1, Dittmer, et al. [66] conducted a study on the modeling and simulation of biogas production at full scale with time series analysis. The authors mentioned that most simulation models deal with complex ADM1, which is known to have many parameters that specifically address biochemical and physicochemical processes. It is reported that the R programming language was used for the study's visualization, modeling, and simulation. Notably, 366 simulations were performed and run, which consisted of the mean absolute percentage error (MAPE), mean absolute error (MAE), and root mean square error (RMSE). The time series analysis reveals a significant negative correlation between solid substrate feed and biogas production. Cross-correlation determined this, confirming the use of solid substrate as a predictor for biogas production. With the 366 simulations, the result achieves a mean MAPE of 14–18%, whereas MAE and RMSE are in the good range of 70 and 60 $m^3 h^{-1}$, respectively. According to the authors, the model delivers a good result with a minimum number of model parameters, as it can produce a high-quality simulation of at least 144 hours.

The simulation of the complete process flow of anaerobic co-digestion, which consisted of pre-treatment of feedstock, biogas upgrading, wastewater treatment, and sludge drying, using SuperPro Designer Software was conducted by Tiong, et al. [16]. During the simulation, hydrogen sulfide is removed to meet a specification of 500 ppm. Wastewater stabilization was also performed to reduce TS, BOD, and COD. For the development of the model, the authors used the following parameters: hydraulic retention time, recycle ratio of sludge, water to food waste ratio, and co-substrate to food waste. These parameters directly or indirectly affect biogas production. Tiong, et al. [16] employed the degradation constant (1/h) and Monod constant (mg/L) as kinetic parameters for the anaerobic digestion simulation in SuperPro Designer. In this case, the carbohydrate (0.0521), protein (0.0333), and fat (0.0292) constitute the components for the degradation constant. From the simulation results, 0.30 LCH4/g of methane, COD removal efficiency (81.5%), and VS removal efficiency (68.9%) were obtained.

3.2. Optimization of Anaerobic Digester

The optimization of anaerobic digesters is important to improve the biogas yield. This means that optimization in relation to process parameters serves as an additional opportunity to maximize biogas production and the efficiency and time spent on the process toward exploring new possibilities [7]. Therefore, identifying and selecting indicators should be considered for successful process optimization. This is because of the information they provide on the condition and functioning of the system [8]. The advantage of monitoring such indicators is that it ensures a smooth process operation and helps detect any malfunctions. The optimization of anaerobic digestion requires several process parameters that need to be considered to ensure a greater yield of biogas as well as an efficient and cost-effective process. Usually, artificial intelligence methods such as neural networks, fuzzy logic, RSM, and design expert systems or software such as RSM are used for optimization and prediction processes [7, 16]. RSM optimization is regarded as an effective approach and tool for anaerobic digestion. Hence, this involves modeling and analyzing the effects of multiple variables in a single variable. The advantage of RSM optimization is that it is time-saving, especially when predicting the coefficients in a mathematical model. To show the effectiveness and efficiency of optimization via RSM, Table 5 presents recent anaerobic digestion studies conducted, indicating the maximum yield of methane and its corresponding optimum parameters.

Table 5.
Selected studies on optimization using RSM.

Waste used	Parameters considered and their optimum condition	Maximum methane conditions (mlCH_4/g VS)	References
Poultry manure + food waste	pH (7); temperature (48.43°C), solid concentration (7.38) and co-digestion (29%)	6.34 ml biogas	Deepanraj, et al. [67]
Cow dung + flower waste	Temperature (50°C); pH (7.2); Waste concentration (100kg); agitation time (5 secs)	568	Gopal, et al. [68]
Rice straw + food waste	C/N ratio (30); pH (7.32); food/microorganism (1.87)	323.78	Kainthola, et al. [69]
Peanut hulls + swine manure	Total solids (5.85%); C/N ratio (34.06:1); Inoculum ratio (%) (30)	686.06	Deng, et al. [70]
Dairy manure + chicken manure + wheat straw	C/N ratio (26.31); feeding composition (42.96:57.04); initial loading (15.90 g VS/L); inoculum to substrate ratio (2.34)	394	Wang, et al. [71]
Food waste + POME	HRT (37.2 days); recycle ratio (0.381); water: feedstock ratio (0.027); POME: Food waste (0.004)	340	Tiong, et al. [16]

Table 5 shows that temperature, inoculum ratio, and C/N ratio are the critical parameters for optimizing anaerobic digestion. High methane yield can be attributed to an increase in the number of volatile solids, which results in high substrate-to-inoculum ratios. Importantly, the high substrate-to-inoculum ratios often affect methane production and limit the performance of methanogenic bacteria. Moreover, pH also influences optimization performance, as seen in Table 5. However, Inayat, et al. [7] state, "One of the important factors leading to improvements in AcoD technology is the interdependence of many components. When only one of these components is researched, the results may not be trustworthy."

Obileke, et al. [72] applied the constrained linear least squares technique to evaluate the performance of a biogas digester under varying operating conditions for optimization purposes. This is one of the optimization techniques or approaches for methane production in the anaerobic digestion of cow dung. The study aimed to address the global challenge of facilitating a decision-making process based on methane production using a predictive model and seeking recommendations. Recall that one of the benefits of the optimization process lies in its assistance in decision-making. The study involves the input parameters (pH, relative humidity, and temperature) as predictors, while the desired response is methane, which was analyzed and conducted using MATLAB. It is imperative to mention that the constrained linear squares used as the optimization tool was made possible based on the custom non-linear model equation employed in the study. Hence, this was reduced to multiple linear regression models with the introduction of the lump input parameter. Contrarily, the optimized lump parameters for methane for the biogas digester were used to produce the optimized predicted response. The study's findings showed that the difference between the optimized model and the general model output for methane production was less than 4%. Therefore, this demonstrates a strong validity as the determination coefficient (R^2) between the modeled and optimized output was 0.968 per the methane volume produced. Based on this, it was recommended that future studies focus on the weaknesses and feasibility of the model, thereby using different volumes of the biogas digester to experiment with predicting the performance.

Optimization of anaerobic digestion is possible in a co-digestion mode of feeding. This was shown in a study by Otieno, et al. [73] on optimizing anaerobic digestion parameters for biogas from pineapple waste with livestock waste in a 6m3 biogas digester. The study optimized the biogas yield as the response (output variable) against the predictor (input variables), such as temperature, pH, and mixing ratio, which was carried out using Box-Behnken Design (BBD). Specifically, the BBD is a Response Surface Methodology (RSM) class commonly achieved through a Design Expert 13 software package. According to Bezerra, et al. [74], the BBD assesses experimental parameters and their interaction, which have a greater significant effect. Moreover, the Expert 13 software was designed to simulate the data obtained from the experiment, thereby establishing the predictive model [75]. The ANOVA tool was employed to assess the statistical significance of the regression model. The maximum biogas yield of 1.98 m3 was reported when the pH was 6.0 – 7.2, the temperature was 30°C, and the mixing ratio was 62.5%, respectively. In analyzing the BBD experimental data, an R2 of 0.99 and P < 0.0001 were obtained for the regression quadratic model equation, which indicates an extremely significant result. Therefore, the results from the study were able to provide the basis for policymakers to make recommendations and strategies for adopting biogas from agricultural waste, which provides green energy and contributes to the economy.

The optimization of pilot-scale biogas plants for mixed food waste with cow dung through anaerobic digestion was conducted by Prithiviraj, et al. [76]. As part of the study, the main objective is to characterize the composition of mixed food waste with cow dung, focusing on the optimum yield of biogas production. However, based on the ANOVA results, it was reported that temperature, pH, and retention time significantly affect the production of biogas ($P < 0.05$). With an optimum biogas yield of 44 ml generated, this tends to be a result of the temperature of 45°C, pH (2.87 – 6.55), and the variation of biogas output peaking in the second ten days.

To determine the optimal conditions for optimizing biogas production in anaerobic digestion, Ingabire, et al. [77] evaluated the impact of inoculum concentration, substrate, and water content (as the input parameters) on the biogas production volume (the output) with the aid of RSM techniques. The Design Expert 13 software, comprised of CCD, ANOVA, and RSM, was used to determine the degree of the input variable, thereby establishing the optimum number of experimental runs (17) to maximize biogas yield. It was reported in the study that the model was significant ($P < 0.05$), and the coefficient of determination (R^2) of 99.9% confirms the good fit of the model with experimental variables. From the study, the biogas yield was said to be a function of operating variables using the linear and quadratic equations, in which all the factors had a significant effect.

Central composition design of the response surface methodology and Python approach were used to optimize the biogas yield from corn cliff and cow dung digestate co-digestion. The study was carried out by Iweka, et al. [78]. The essence of the study was to assist and guide the facility operators in facilitating the decision-making process related to biogas, thereby integrating the obtained model into their operation. Thirteen experimental runs were generated at different substrate-to-inoculum (S/I) ratio conditions and HRT as the input variables under a mesophilic temperature range of 25 – 33°C. The optimum cumulative biogas yield from the study was 6.1883 L, obtained at a mixing ratio of 0.65 in 37 days (HRT). Both factors are known to affect the volume of the cumulative biogas yield and significantly impact the anaerobic digestion process, as shown in the ANOVA result. In addition, R^2 of 0.9966 indicates that the obtained model from the study accounts for 99.66% of the variability observed in the model response. This shows the reliability of the result. Notably, the R^2, adjusted R^2, and predicted R^2 is close to 1, indicating that the experimental results are reliable and consistent. For the model's P and F-values, the findings reveal that the P-value > 0.05 (insignificance). The F-value of 0.80 implies a lack of fit, which is not significant relative to the pure error. In contribution to Iweka, et al. [78] study, Falowo, et al. [79] mentioned that a non-significant lack of fitness is good because it describes the model fitness. Therefore, the result of the study shows that both CCD and Python can model the production of biogas with high accuracy and should be recommended.

Table 6.
Review the summary of selected optimization studies of anaerobic digestion for energy generation from the literature.

Substrate used	Predictors	Desired response	Optimization techniques	Results/findings	References
Cow dung	pH, global irradiance, relative humidity, Temperature	Methane	Constrained least square (CLS)	$R^2 = 0.96$; Maximum methane yield = 0.24 m^3.	Obileke, et al. [72]
Pineapples + Livestock	Temperature, pH, Mixing ratio	Biogas	Response surface methodology (RSM) and Box Behnken design (BBD)	Maximum biogas yield = 1.98m^3; pH = 6.0 – 7.2; P-values < 0.0001; F- value = 1.19; $R^2 = 0.99$	Otieno, et al. [73]
Water hyacinth + fish waste	Substrate ratio; inoculum concentration and water content	Biogas	Response surface methodology (RSM); Analysis of variance (ANOVA) and Central composition design (CCD)	Maximum biogas yield = 690 mL; Substrate ratio = 25:75 g; inoculum concentration = 15 g; water dilution = 95 mL	Ingabire, et al. [77]
Corn chaff + cow dung	Mixing ratio (substrate-to-inoculum) and HRT	Biogas	CCD + RSM + Python	Biogas yield = 6.1883 L; Mixing ratio = 0.65; HRT = 37 days	Iweka, et al. [78]

The development of mathematical and intelligent models is an effort to address the inadequate understanding of microbial, kinetic, and physiochemical processes related to the anaerobic digestion process. This was revealed in the study by Olatunji, et al. [80] on the evolutionary optimization of biogas production from food, fruit, and vegetable waste. In differentiating the mathematical and intelligent models, the authors mentioned that the mathematical model provides near-optimal solutions and is time-consuming, expensive, and very demanding, whereas the intelligent model is limited by its low predictive performance and capability. A genetic algorithm (GA) was used to optimize an adaptive neuro-fuzzy inference system (ANFIS) for the cumulative biogas production (targeted output) using seven input variables (OLR, VS, pH, HRT, Temperature, retention time (RT), and reaction volume (RV)). The choice of using the adaptive neuro-fuzzy inference system is based on its combination of fuzzy inference linguistic transparency with the self-learning capability of the neural network, as pointed out in the study. From the study, the authors reported that 35% and 31% of HRT and VS influence the cumulative biogas production prediction. In contrast, the pH contributes 22% to the biogas cumulative production (output). On the other hand, the volume of the reactor was regarded as the least influential to the output. Without any doubt, the significance of HRT is due to its impact on other variables (temperature and substrate composition), as mentioned in the studies by Sandhu and Kaushal [81] and Tabatabaei, et al. [82]. In this case, as the activities of bacteria reduce, the HRT also reduces, and more HRT will lead to a larger biogas digester with higher costs and low efficiency. The findings from the study are a guide and serve as an effective tool for the upscaling of anaerobic digestion, as well as techno-economic studies based on efficient energy utilization.

3.3. Recent Studies on Process Simulation and Optimization of Anaerobic Digestion

To simulate the complete process flow of anaerobic digestion, Tiong, et al. [16] conducted a study on the simulation and optimization of anaerobic co-digestion of food waste with POME for biogas production. Their study consisted of the pre-treatment of feedstock, biogas upgrading, wastewater treatment, and sludge drying. Part of their study's methodology was the involvement of Super Pro Designer Parameters. This includes HRT, the recycling ratio of sludge water to food waste ratio, and the co-substrate of food waste. These are said to affect the performance of the anaerobic digester. With the aid of design expert software, the RSM was used to investigate the effect of the independent variables (HRT, recycle ratio of the digester, water: substrate ratio, and POME: food waste) as the predictors, whereas the flow of methane, COD, and VS removal efficiency as the response variables. During the digestion of 25,000 kg/h of feed in the study, the optimized values for HRT, recycle ratio, water to feedstock ratio, and POME to FW ratio include 37.2 days, 0.381, 0.027, and 0.004, respectively. This results in a methane yield of 0.30 L CH4/g of COD removed, with COD and VS removal efficiencies reported at 81.5% and 68.9%, respectively.

Inayat, et al. [7] conducted a review study on process simulation and optimization of anaerobic co-digestion. The review provides an overview of the operational parameters in the anaerobic co-digestion process, including the modeling, overall process optimization, and standard software used for optimization (Aspen Plus, SuperPro Designer, Biowin, CFD, and MATLAB). In addition, the review addresses the design development and optimization framework for biogas production, thereby considering numerous aspects. The authors' findings from the review indicate that using RSM for simulation and optimization of anaerobic digestion predicts the optimum maximum methane yield. Furthermore, the optimization methods efficiently assist in modifying the ratio, concentration, and particle size of the substrate and various residues. The review abstract concluded that temperature, substrate concentration, inoculum ratio, and C/N ratio are the most significant optimization parameters and should be recommended.

Ganeshan and Rajendran [20] developed a modified Hill model using MATLAB (V2021b) to predict biomethane production with time series to perform a dynamic simulation and optimization of anaerobic digestion (batch and continuous). The time series-based modeling employed in the study is scarce in the literature, thereby providing a fundamental understanding of process fluctuation in anaerobic digestion. Usually, the modified Hill model forecasts the dynamic behavior of anaerobic digestion. However, in their study, the model used a set of differential equations to characterize the various stages of anaerobic digestion. The model input used in the study includes organic loading rate (OLR), reactor volume, and operating temperature. On the other hand, the monitoring parameters are death rate and rate kinetics. During the development of the model, certain assumptions were made, such as constant reactor stirring, volume of the reactor, and constant temperature. Considering the deviation of the literature Haugen, et al. [83]; Pathmasiri, et al. [84] and Saeed, et al. [29], the model developed in the study by Ganeshan and Rajendran [20] reported less than ± 7.6%. This was said to confirm the accuracy and robustness of the model. The statistical analysis revealed no significant difference between the literature and simulation, verifying the null hypothesis. Interestingly, optimizing the loading rate yielded maximum methane production, thereby showing stability from an operational perspective. The study has proved that real-time operations of the anaerobic digesters and laboratories estimate the best region of operation regarding loading rate and biogas yield.

4. Limitations of the Study

The hydrodynamic conditions and parameters of digestate in the anaerobic digester, such as the viscosity and pH, remain unknown. In this case, the incorporation of mixing is needed to overcome the resistance associated with mass transfer. This is because, with higher total solids content, the viscosity of digestate increases, thereby increasing mass transfer resistance for the diffusion of gases. The application of models in anaerobic digestion, focusing on their flexibility and adaptability as well as processing time, was considered in the study. Models are regarded and used based on their predictive capabilities by approaching different designs and operating conditions, thereby improving and optimizing biogas yield. This might not be considered in detail and exhaustively in the study, but it requires further study. Additionally, despite the study's benefit in analyzing, designing, testing, and optimizing the anaerobic digester system, its accuracy, validity, and scalability need to be widely explored as they impact and influence the study's findings and methodology.

5. Recommendation and Future Research

According to Rozakis, et al. [85], studies in relation to process optimization and simulation of an anaerobic digester provide new, innovative, and additional approaches in the biogas arena, thereby accomplishing the desired biogas sector goals. Process optimization relating to parameters, mathematical modeling, and simulation are recommended to improve economic viability and higher biogas yield, particularly for anaerobic co-digestion. Moreover, for the benefit of the policymaker, the study will promote the efficient commercialization of an anaerobic co-digestion reactor based on the optimization and simulation findings. Therefore, studies of this nature encourage and assist local communities in improving biogas production, thereby increasing the acceptance of biogas technology [21].

Thus, some of the suggestions that might require further research include the following:

- Simulations in the numerical area need to be conducted because they will assist researchers in optimizing parameters and predicting biogas production under different conditions. This will provide estimates and evidence and significantly contribute to the body of knowledge.
- Further studies are required to improve the accuracy of BioModel, especially for the description of certain inhibition phenomena. This will be done using optimized parameters to expand the applicability or simulate manure and wastewater-based co-digestion (via mesophilic or thermophilic conditions).
- ADM1, for example, has been implemented in different commercial software (GPS-X, SIMBA, and AQUASIM) and programming languages (JAVA, FORTRAN, and C). However, a good understanding and knowledge of engineering principles and in-depth information on the input parameters for modeling, simulation, and optimization of biogas processes need to be carried out.
- There are still research gaps in optimizing the co-digestion of the anaerobic process in relation to the environmental and time-based fluctuations of the feedstock for the simulation of biogas yield. To this effect, studies should be conducted to combine the biogas model with a multistage mechanism of anaerobic co-digestion and parameters that influence the yield.
- The high organic load associated with substrates of different characteristics makes process modeling more extensive in anaerobic co-digestion than in mono-digestion. With that in mind, several reviews, including the present one, have recommended further consideration of a new simulation model to deal with the system's performance, organic loading rate, and co-digestion content in an effort to optimize biogas yield.

6. Conclusions

This review presents the recent advances in maximizing biogas yield in relation to the simulation and optimization of anaerobic digestion. Various optimization techniques and simulation tools, as well as their application in anaerobic digestion, coupled with the description and development of the process model, were exhaustively detailed. Additionally, modeling anaerobic digestion using models and simulation software was critically reviewed, referencing their advantages and disadvantages. From the review, it was established that models are employed based on their predictive capability under different operating conditions and parameters as a way to improve biogas yield. To maximize biogas yield, an important aspect to focus on is the control of process parameters. Previous studies have concentrated on publishing original research in terms of experimental studies. Hence, a review of their findings and applications remains limited and unclear. Part of the findings from the review emphasized that the processing time for anaerobic digestion can be shortened through process modeling. Furthermore, the RSM was revealed to be the most effective approach and tool for optimization techniques. This is attributed to its handling of multiple variables in a single variable in terms of modeling and analysis, along with advantages such as time-saving.

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