

## Review Article

# Biogas Production Optimization in the Anaerobic Codigestion Process: A Critical Review on Process Parameters Modeling and Simulation Tools

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Many operational parameters, either discretely or collectively, can influence the biodegradation performance towards enhancing biogas yield and quality. Among the operating parameters, organic loading rate (OLR), inoculum-substrate ratio, and carbon-nitrogen ratio (C/N) are the most critical parameters in the optimization and enhancement of biogas yield. Optimization of the biogas production processes depends on the ability of anaerobic microorganisms to respond to variations in operational parameters such as pH, redox potential, and intermediate products to enhance the biogas yield. This review article focuses on the role of process parameters, kinetic models, artificial intelligence, Aspen Plus (AP), and anaerobic digestion model no. 1 (ADM1) in optimizing biogas yield via an anaerobic codigestion (AcoD) process. The review showed that biomaterials codigestion upgraded biogas yield to the extent of 400%, and organic removal efficiency reached up to 90% compared to a single substrate. In addition, the current work has verified that the kinetic model is the most effective tool for signifying that the hydrolysis phase is the rate-limiting step, whereas AP is the most effective tool in the design and optimization of the AcoD process parameters. The reviewed kinetic and AI models show strong correlation values ranging from 0.931 to 0.9991 and 0.8700 to 0.9998, respectively. The AcoD system involves complex chemical reactions, but AP might have limitations in representing such complex chemical processes with nonideal behavior and complicated reaction mechanisms. The design and optimization of AcoD with reliable input parameters are highly limited or nonexistent. The AcoD process design with AP opens fresh research opportunities, including improved efficiency, finding appropriate retention time, and saving time, as well as finding the optimum biogas yield. This review article gives an insightful understanding of AcoD process parameter optimization and valuable strategies for policy development enhancing sustainability in the biogas sector.

## 1. Introduction

The global energy crisis, fast population growth, and rapid depletion of nonrenewable energy sources coupled with global warming caused by greenhouse gas (GHG) emissions, particularly carbon dioxide (CO<sub>2</sub>), press the concerned bodies to find an environmentally sound alternative energy source to reduce the dependence on fossil fuels [1]. Bio-energy can be obtained from any biologically decomposable organic matter, such as plants or animals, terrestrial plants,

aquatic plants, wastes from wood processing, organic fractions of municipal solid wastes, animal manures, crop residues, sewage sludge, and debris from forestry, are only a few examples of biomass energy sources [2]. As compared to other waste treatment technologies, biogas plants emit fewer GHG into the atmosphere. Anaerobic digestion (AD) technology has received widespread global acceptance and appears to have strong prospects [3–5]. The use of biogas technology in the industry and at home, as well as fertilizers in agriculture, is a wonderful example of a circular green

economy. It also minimizes the use of nonrenewable fuels, including wood and charcoal, and indirectly helps to conserve the forests and biodiversity resources. Therefore, waste conversion into bioenergy is just more than an issue of clean energy production. It has a broader impact because it minimizes groundwater pollution [6], solves a waste disposal problem and its associated costs, and reduces greenhouse gas emissions by moderating methane emissions [7]. The treatment of wastewater or liquid/solid waste from livestock contributes to the reduction of pollution in lakes and rivers [8].

AD is the biochemical decomposition of organic materials by groups of archaea under an oxygen-free environment to produce gaseous compounds, mainly consisting of 50–75% methane [9]. However, anaerobic monodigestion does not produce sufficient biogas yields due to several issues, such as nutrient imbalance, fluctuations in feedstock, inhibitory compounds, lack of diversified microbes, and the effect of operating conditions [10]. AcoD offers an opportunity to overcome the failures of monodigestion by simultaneously degrading more than two substrates in one bioreactor. In addition, AcoD may serve the purpose of improving system stability and neutralizing toxic compounds [11]. The synergistic effects of AcoD encourage microbial consortia, better nutrient balance (right C/N ratio and delivery of trace elements) [12], provision of the needed amount of moisture for the bioreactor [13], increasing the OLRs [14], and improving the speed of biodegradations [15]. Despite its complexity, several computational models have been developed to symbolize the biochemical transformation of organic waste during the AD process to predict and optimize the mixing ratios and OLRs, avoid process variability and costs, lower the energy loss [16, 17], and reduce the process time to maximize biogas production [18–20]. The mathematical models used to describe the kinetic parameters include the Monod model, first-order kinetic, modified Gompertz models [21], and transference function [22]. In addition, the models applied to forecast and simulate the mono AD process include artificial intelligence (artificial neural networks (ANNs), ant colony optimization (ACO), genetic algorithms (GAs), and particle swarm optimization (PSO)), and hybrids of these models [23, 24]. Furthermore, a variety of different common software programs have been applied to simulate and optimize the AcoD process, such as Aspen Plus (AP), AQUASIM, ADM1, and sewage treatment operation analysis over time (STOAT) [20, 25, 26]. Among the relevant software tools, ADM1 and Aspen Plus are found to be the most favorable in predicting suitable working environments. These interactive and reliable models offer better data optimization and process simulation around the AcoD system [20].

The general objective of this work is to comprehensively review and analyze the experimental and modeling approaches used in the optimization of biogas production through an AcoD system with better efficiency. While exploring the previous works, evolution, and predictions of the AD process in an attempt to improve biogas yields, much focus is given to process parameters, codigestion, modeling, simulation, and optimization. The present review is unique

in the sense that none of the previous review articles integrated biogas production process parameters and simulation models as a way forward for understanding biogas yield optimization. This review adds an insightful body of knowledge besides opening up new research opportunities in the biogas field. The output of the current work can benefit households and medium-scale and commercial-level biogas plants in adapting to the technology. Efficient biochemical conversion can greatly help increase the acceptance and adoption of biogas technology, accelerating the global shift towards green energy technologies. This shift can significantly contribute to climate change mitigation in the current context.

## 2. Stages of the Anaerobic Codigestion Process

The concept behind the AcoD process is complex, as the biological breakdown of organic waste is performed in a multistep process by groups of anaerobic microbes in an oxygen-limited condition. Biogas is the end-product of AD, which is composed of 50–75% methane the energy carrier, 25–50% CO<sub>2</sub>, and other trace compounds of hydrogen sulfide, nitrogen, ammonia, and hydrogen [9]. The anaerobic conditions include hydrolysis, acidogenesis, acetogenesis, and methanogenesis. Figure 1 represents the steps involved for groups of anaerobic microbes to produce biogas from waste materials [10].

In the first step (hydrolysis stage), extracellular enzymes released by microorganisms degrade long-chain polymers and other complex organic materials, such as carbohydrates, proteins, and lipids, into their respective simple forms [27]. In the acidogenesis step, most hydrolysis products are still macromolecules which must be transformed into smaller units such as acetic acid. In the second stage, acidogenic bacteria convert simple sugars, amino acids, and fatty acids to acetate, CO<sub>2</sub>, and other trace products. Also, volatile fatty acids (VFAs) such as acetic acid, butyric acid, propionic acid, and other organic acids are produced in this stage [28]. Furthermore, the organic compounds are converted to acetone, glycerol, and alcohols. Acidogenesis is a fast exothermic step that occurs during AD. In a well-functioning anaerobic system, about 70–80% of the hydrolysis products are converted to hydrogen, CO<sub>2</sub>, and acetate, which are easily available to methanogenic microbes. In comparison, the remainder of 20–30% is translated to other intermediate products [29]. In the acetogenesis stage, either hydrogen-producing or hydrogen-consuming agents produce acetate. Hydrogen-producing agents oxidize the acids to acetate. This oxidation reaction produces electrons, which are transformed to H<sup>+</sup> to form H<sub>2</sub> and formate [30]. In the final stage, methanogenic microbes use acetate, H<sub>2</sub>, and CO<sub>2</sub> in the synthesis of methane. This process occurs in one of the two ways: acetoclastic methanogenesis or hydrogenotrophic methanogenesis [31]. In the former approach, acetate is the main feed for producing methane, but in the latter method, hydrogen is engaged to decrease CO<sub>2</sub>. Adjusting the ideal pH value is crucial to guarantee maximum activity for the acidifying and methanogenic bacteria [10]. For example, the methanogenesis step should occur at a pH of over 6.6, ideally

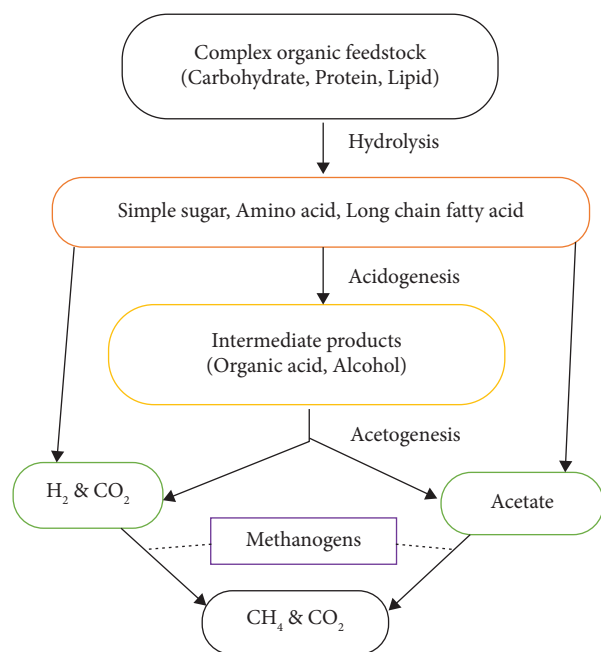


FIGURE 1: The steps involved in biogas production (modified from [10]).

between 6.8 and 7.2, to produce the maximum amount of methane [30]. Caruso et al. [32] identified some conditions that can delay bacterial growth and activity, including a shortage of nutrients and the existence of inhibitory chemicals such as sulfide, which causes a drop in pH and VFA accumulation.

### 3. Process Parameters

Numerous factors influence the efficiency of anaerobic digestion and the feasibility of codigestion in situations where adequate management is required to avoid reactor failure. Chemical compositions of the substrate, mixing, inoculum-substrate ratio (ISR), biological oxygen demand (BOD) and chemical oxygen demand (COD), OLR, substrate mixing ratio, nutritional balance, hydraulic retention time (HRT), and operating temperature in the digester are a few of the key factors that have a significant influence on performance during codigestion. These factors are also further evaluated, reviewed, and discussed in the following sections to obtain a better understanding of a way forward, while referring to Tables 1 and 2. The summarized optimal operating conditions are also highlighted.

**3.1. Chemical Composition of Substrates.** Chemical composition refers to the specific elements, compounds, and organic contents present in the substrates that are being used as a feedstock for biogas production. The specific chemical compositions of organic materials may vary depending on numerous factors, including the waste or biomass type, its origin or source, and its regional location [44]. Typically, substrates utilized in the generation of biogas comprise the following components: water content provides the necessary

moisture for microbial activity and the AD process. Inorganic components, such as salts and minerals present in organic materials, can influence alkalinity, pH, and buffering capacity. Organic matter (fractions), which includes carbohydrates, proteins, lipids, and other complex organic compounds [21], constitutes the primary energy source for microbes [10]. Essential nutrients, including nitrogen [45], potassium, phosphorus (P), sulfur, and trace elements such as magnesium, iron, and calcium, are necessary for microbial growth and metabolism. The chemical composition of substrates has significant effects on the process parameters, including OLR, pH, and alkalinity [46]. Thus, understanding the specific composition of substrates is essential as it aids in assessing the suitability of substrates for methane production, forecasting biogas production potential, and optimizing process parameters. In addition, by carefully picking and mixing the substrates, it is possible to obtain upgraded nutrient balance, higher biogas yields, and better overall process performance in AcoD systems.

**3.2. Agitation/Mixing Rate.** Agitation/mixing rate refers to the intensity at which the organic materials inside the digester are mixed. It involves the movement of the organic waste and the inoculum to create a well-mixed environment, promoting efficient biogas production [47]. Mixing stimulates contact between microorganisms and substrates and provides uniform temperature distribution in the digester. Adequate mixing can reduce foaming caused by floating fat, filamentous microorganisms, or by adhering to gas bubbles. Mixing in the bioreactor is aimed at solid accumulation, floating layers, and the release of the entrapped biogas in the digestate. Adequate contact between nutrients and microorganisms requires proper mixing. As they have negative influences on biogas production and higher power consumption, continuously mixed digesters are no longer encouraged. It has been reported that biomethane production increased by 220% with 160 rpm bidirectional mixing [48]. Mixing may be proficient by employing hydraulic (liquid recirculation), mechanical (manually or using a mixer), and pneumatic (recirculation of gases) systems at various frequencies (continuously or intermittently several times in an hour during a day) and strengths (intermittent, gentle, and rotation speed) [49].

The agitation/mixing rate can vary depending on parameters, including the digester size, design, substrate characteristics, and process requirements [50]. It is normally attained using mechanical pumps, stirrers, or recirculation systems that form turbulence and circulation inside the digester. The optimal mixing rate should be balanced to ensure enough mixing without high energy consumption. A high agitation rate may increase energy demands and stress on microorganisms [51], while a low agitation rate may result in insufficient substrate contact and partial digestion [48]. Generally, even though the prominence of mixing to enhance process performance is prominent by several investigators, the optimum mixing practice is still a questionable issue, so it is difficult to tell the optimum mixing intensity because sufficient mixing is subject to a large number of parameters, which vary for all the experiments.

TABLE 1: Optimum ranges of operational parameters for the optimization of the anaerobic codigestion process.

Operational parameter	Optimal values	References
ISR	>2:1	[33]
C/N ratio	20–30:1	[34]
pH	6–8.50	[30, 35]
OLR	1–6 g VS or COD/l.d	[32, 36]
Temperature	Cryophilic (15–25°C), mesophilic (35–40°C), and thermophilic (50–60°C)	[37]
VFA/TA ratio	0.20–0.40	[14]
TA	1000–5000 mg CaCO <sub>3</sub> /l	[27]

d, day; TA, alkalinity; l, liter; mg, milligram; g, gram.

**3.3. Inoculum-Substrate Ratio.** The ISR refers to the proportion of inoculum (also called seed material) to the substrate in AD processes. The inoculum is a mixture of microorganisms, which kick-start the reaction process by providing the essential microbes and enzymes to degrade organic waste. To obtain the maximum biomethane production rate and high biomethane yield, the correct balance between the substrate and inoculum is crucial [21]. The ratio decides the initial microbial community and its ability to degrade the substrate biologically [52]. Ideally, the methane yield might be independent of the ISR, and the ISR only affects the reaction rates. However, experimental data indicate that ISR may affect both due to the real evidence that the proportion directly affects microbial growth patterns. Too low ISR below the optimum value may prevent the induction of the enzyme required for biodegradation and thus a small amount of biogas is produced, which could affect the conversion and methane yield. It is suggested that for substrates with poor organic matter concentration that is not easy to degrade, a substrate-inoculum ratio could be set at higher ranges over substrates with high organic compositions that are easily biodegradable. The German standard, VDI 4630, recommends a substrate-inoculum ratio of less than 0.50 [33]. For example, Ibro et al. [23] evaluated the effect of the inoculum-substrate ratio on biogas production performance, and the highest biodegradability and biogas production was attained at an ISR of 2. Despite their potential to initiate the start-up of the biochemical reaction, it is not easy to compare kinetic parameters due to the complex nature of each experimental setup (inoculum source and temperature) [53].

**3.4. Biochemical Oxygen Demand and Chemical Oxygen Demand.** BOD is a parameter that is used to measure the oxygen consumed by the microorganisms to degrade the organic matter in the wastewater. It indicates the amount of oxygen required to oxidize the organic material existing in organic wastewater biochemically [54]. COD is used to evaluate the amount of organic matter in waste, including the oxygen demand formed by biodegradable and non-biodegradable organic materials. Therefore, COD values are larger than BOD [55]. In addition, COD is a useful indicator of the biogas conversion efficiency of the bioreactor. The quantity of biogas yield increased gradually with the increment of COD concentration [56]. AD includes most alternatives as a former treatment of waste on environmental

and energy security, potentially leading to COD and BOD removals as high as 90 and 95% at optimum conditions [56]. For a given sample, the COD value after biodegradation specifies only the amount of the nonbiodegradable organic matter. Therefore, it is obvious that the difference in COD before and after microbial degradation ( $\Delta\text{COD}$ ) equals the BOD value because both represent the amount of biodegradable organic materials. In addition, COD can improve the deficiencies of BOD, which is defined as the oxygen amount consumed when organic matter in waste is decomposed by external oxidants under certain conditions [55]. The intensity of the chemical composition of organic material directly influences the concentration of the biogas production. In addition, COD balance indicates the synergistic effect of codigestion due to a blend of supplement materials (available here). All experiments indicated that the results of COD and BOD are proportional to the biogas output of the bioreactor. So, the nature and composition of the organic matter available in the waste may directly affect biogas production [57].

**3.5. Carbon-Nitrogen Ratios.** In AD systems, the C/N ratio refers to the ratio of carbon to nitrogen content in the organic materials being treated. The C/N ratio indicates the level of the nutritional content of feedstocks that are significantly exposed to microorganisms. To improve process performance and stability, the C/N ratio must be optimized, like other parameters. The system becomes unstable, and biogas generation falls as the C/N ratio deviates from the ideal C/N ratios. Thus, identifying C/N levels is important for decreasing or eliminating ammonia build-up during the AD process [34]. A low C/N ratio implies insufficient carbon content or nitrogen underuse, which causes an excessive ammonia concentration, phenolic compounds production, and a drop in pH [58]. Carbon-rich substrates such as kitchen wastes and energy crops can be added to enhance biogas yield. In contrast, if the C/N ratio is too high, it indicates a deficiency of nitrogen relative to carbon, which can slow down the microbial activity leading to a longer retention time in the reactor and lower biogas production rates [59]. In this case, nitrogenous substrates, such as animal dung and poultry droppings, can be employed to increase biogas production. Table 1 shows the ideal C/N ratio, which is adequate to maintain the system stability and satisfies anticipated energy and nutritional needs for the efficient metabolic activities of the microbial groups [60].

TABLE 2: Summary of operative parameters for AcoD optimization and their achievements in terms of methane yields.

Substrate	Mixing ratio	C/N ratio	OLRs	Improvements	References
Empty fruit bunches (EFBs) and palm oil mill effluent (POME)	—	45	—	The cumulative CH <sub>4</sub> increased from 0.17 to 2.03 l	[38]
Chicken manure (CM), dairy manure (DM), and rice straw (RS)	—	25 and 30	—	Maximum CH <sub>4</sub> yield and reduction of ammonia inhibition were observed	[39]
FW/cow manure	2.5	—	11.9 g COD/l/d 0.06 kg VS/m <sup>3</sup> <sub>h</sub>	441 ml CH <sub>4</sub> /g VS	[40]
Cabbage, cauliflower, and food waste	0.36 : 0.64	45	—	Maximum CH <sub>4</sub> and high biodegradability (98%) was attained	[41]
Sugarcane bagasse (SB) and fruit-vegetable waste (FVW)	30 : 70	—	—	CH <sub>4</sub> yields increased by 56% over monodigestion of SB	[42]
WH/FW	40 : 60	21.47	—	Enhanced biogas volume by 55.2% with maximum biodegradability of 89.3% compared to digesting WH alone	[21]
R. Okamura and OMSW	1 : 3	27.4	—	Improved CH <sub>4</sub> yields 177% over R. Okamura treating alone	[22]
CH/WH/FW	25 : 25 : 50	23.7	—	Biogas volume improved by 179.7% with maximum biodegradability of 89.22% over CH testing alone	[43]

h, hours; kg, kilograms.

For example, Lama et al. [22] codigested alga *Rugulopteryx okamura* (*R. okamura*) with olive mill solid residues (OMSW) to identify their feasibility for biogas production. They observed the maximum methane yield for the mixture at a C/N ratio of 27.4, enhancing the methane yield of macroalgae alone by 157%. In other work, biogas yield improved by 179.7% at a C/N ratio of 23.7 for codigestion of coffee husk (CH), water hyacinth (WH), and food waste (FW) [43]. Furthermore, operative parameters, such as pH, temperature, and factors such as VFA and ammonia concentrations may extremely influence the carbon and nitrogen contents in a feedstock [61]. Thus, choosing the right C/N ratio is challenging because various factors, including substrate type, trace elements, chemical components, and biodegradability, might affect the ideal values.

**3.6. Organic Loading Rates.** OLR is another important operating parameter in AD processes that determines a bioreactor's capacity to treat organic waste efficiently. OLR refers to the amount of organic content (usually measured as COD) that can be fed into the reactor per unit volume within a given time (e.g., g COD/ml/d). Under the continuous mode of the AD process, it is the daily amount of organic substrate added to the anaerobic reactors. Increasing OLR promotes microbial activity, which may improve biogas production [62]. However, feeding the substrate into the digester without considering the optimum OLR mentioned in Table 1 resulted in a biogas volume reduction. In the overloaded biodigester, the free motion of microorganisms would be restricted, and they have an excessive concentration of VFA, which may affect the CH<sub>4</sub>-producing methanogens [63]. For example, increasing OLR showed a drop in biogas production by 168% [14]. Low loads (introducing little organic material) cause the digester to become alkaline and produce poor biogas [13]. The optimal OLR for an anaerobic reactor depends on some factors, including the feedstock type, reactor configuration, and HRT. In addition, the operating temperatures, substrate composition, and biodegradability may affect the OLRs. AcoD allows for the adjustment of the overall composition of the substrate to optimize the OLR and attain maximum biogas volumes. For instance, the maximum methane yield and the highest biodegradability of 98% were obtained from the mixture of cabbage, cauliflower, and food waste at an OLR of 0.06 kg VS/m<sup>3</sup>/h [41].

**3.7. Hydraulic Retention Time and Temperature.** The average time interval that a soluble organic compound (sludge) remains in a biodigester is referred to as the hydraulic retention time. HRT may significantly influence microorganisms and biogas yields. Classical biodigesters require long HRTs of 20–200 d and large areas, and the biogas is released directly into the atmosphere, contributing to greenhouse gases [64]. This problem can be overcome by using a fast cooker with a small footprint and short residence time. A short HRT helps reduce capital costs and bioreactor volumes but leads to the washing away of active microbes. Different studies indicate that HRT influences degradation

efficiency, methanogenesis, and microbial community distribution. For example, the AcoD experiment performed at the HRT between 10 and 20 d showed a removal efficiency of the VS and COD up to 90% due to the synergistic effects of codigestion of cattle manure with other biowaste matter [32]. In addition, the review report showed 77% high-quality biogas and 87% COD removal at a lower retention of 12 h [61].

In addition, the time it takes for an anaerobic digestion to break down the waste depends on environmental factors such as temperature, which refers to the operating condition of the AD system. Temperature is an important parameter affecting the methane content in biogas, biogas production rate, and system performance. The AD process can operate primarily under three different temperature conditions, such as cryophilic (15–25°C), mesophilic (35–40°C), and thermophilic (50–60°C) [37]. The biogas yield produced in thermophilic anaerobic digestion conditions was slightly higher than that produced in mesophilic conditions. At high temperatures, the production of H<sub>2</sub> from the oxidation of organic acids becomes energetically more favorable, while the consumption of H<sub>2</sub> due to hydrogenotrophic methanogenesis becomes less clear [65]. Mahanti and Ghatak [66] evaluated the effects of temperature on kinetic rates of AD of lignocellulosic biomass. The results specified that the biogas production rate increased with increasing temperature. In another experiment, a 400% increment in biogas generation was reported under mesophilic conditions when 4% of glycerol was codigested with pig manure, compared to monodigestion [67]. However, instability issues might crop up during thermophilic operation. Another limitation is the additional heating expense in thermophilic digestion [10]. Franqueto et al. [68] also investigated the influence of temperature variation on biogas production from codigestion of rice straw and animal waste in bench-scale bioreactors. Regarding temperature, all bioreactors were shown to adapt to the mesophilic and thermophilic conditions due to the synergism between the substrates tested. Mesophilic conditions were determined to be the most promising for biogas generation due to the higher stability and lower energy consumption. In addition, Rahman et al. [69] experimented on codigestion of poultry manure and kitchen wastes to assess the effects of temperature and mixing ratio on biogas production under room temperature (28°C) and mesophilic conditions (37°C) and maximum biogas yield was achieved at mesophilic condition. They suggested that codigestion could be a promising way to increase methane yields by ensuring nutrient balance, reactor stability, and buffering capacity under controlled mesophilic temperature.

**3.8. pH and VFA/TA Ratios.** The pH, VFA, and VFA/TA (total alkalinity) ratios are the most important factors that require measurement to determine the stability and performance of the AcoD process for maximum biogas generation. The pH value is one of the operational parameters that influence microbial activity and methane yield. It is an indicator of biodigester stability. The optimum pH value depends on the type of anaerobic microbes that participate

in the system. In the process of producing methane, most bacteria prefer a neutral pH. Kornaros et al. [70] experimented with the AcoD of CM and sorghum aimed at studying the influence of initial pH value on  $\text{CH}_4$  and  $\text{H}_2$  production in a two-stage digester. They achieved the highest  $\text{H}_2$  yield of 0.92 mol  $\text{H}_2$ /mol carbohydrates consumed at pH 5. Furthermore, a crucial indicator of the stability of an anaerobic bioreactor is VFA. The VFAs are organic acids produced during the acidogenesis phase of AD, primarily including propionic acid, acetic acid, and butyric acid that serve as precursors for  $\text{CH}_4$  production. In biodigester, excessive VFA formation can lower pH levels, which can affect active methanogens and disrupt the stability of the digester. Notably, undesirable VFA accumulation occurred because of active microbial washout, digester overfeeding, or formation of inhibitory compounds in the system. In addition, when the amount of water required for microbial conversion is insufficient, it leads to high VFA or ammonia production. In such conditions, codigestion with a competitive material prevents fluid dispersion routes and drastically reduces the severe rise and production of toxin compounds in the slurry [71]. A buffering capacity of a molar ratio of at least 1:1.4 of VFA to bicarbonate is necessary to ensure a stable and well-buffered digesting process [60].

TA is defined as an aqueous solution's capacity to neutralize acids. Compared to direct pH measurement, it is a more responsible indicator of digester imbalance. Anaerobic microbes produce TA that prevents the pH drop in the form of  $\text{CO}_2$  and bicarbonate. For optimal methane production, alkalinity should be maintained within the range shown in Table 1 [27]. The VFA/TA ratio is a critical parameter, which is also used to assess the overall performance of the AcoD process. It provides valuable information about the acidification and buffering capacity of the digester. In an anaerobic system, a loss in alkalinity or an increase in the amount of VFA causes a rapid drop in pH [72]. Yang et al. [35] codigested maize stalk and swine manure to evaluate the influence of initial pH on the process stability and methane ( $\text{CH}_4$ ) production under thermophilic conditions for 35 days. They confirmed the VFA/TA ratio of 0.10-0.30 and the initial pH of 6.81 as optimum anaerobic reaction conditions for methanogen activity. The VFA/TA ratio is the early detection of process failure if the optimum range defined in Table 1 is exceeded [14]. Table 2 summarizes some important process parameters for AcoD optimization and their achievements.

**3.9. Digester Dimensions.** The biogas digester dimensions include parameters such as height, length, diameter, width, or depth [50]. These measurements give evidence about the extent and capacity of the anaerobic digester, which is essential for deciding the OLR and the biogas generation potential. A particular waste stream treatment requires an appropriate reactor configuration. The main feedstock qualities, specifically the organic loading rate and total solids content, are used to determine which digester type is

appropriate for maximum biogas production [50]. Thus, to construct a biodigester, the three main requirements must be addressed: managing a high OLR continuously, having a short HRT, and producing a large volume of methane-rich biogas. Upflow anaerobic sludge blanket (UASB) reactors [73], plug-flow systems, anaerobic sequencing batch reactors (ASB3Rs), Anaerobic Baffled Reactor (ABR), anaerobic filters, and tubular reactors are among the other biodigester types currently available. Fu et al. [73] compared the effects of the reactor configuration on biogas production, such as a leaching bed upflow anaerobic sludge blanket (UASB) and a semicontinuous continuously stirred tank reactor (CSTR). The results showed that the specific methane yields were 370 and 248 ml/gVS in the CSTR and the leach bed-UASB processes, respectively, after a processing time of 29-30 days. CSTRs are high-rate digesters that are perhaps the most utilized digesters to handle slurries with a total solids content of 5-10% in biogas production. As mentioned above, most reactor configurations have been studied to accomplish a high OLR. For instance, an anaerobic membrane bioreactor with internal circulation and a superhigh-rate reactor are some of the innovative configurations publicized to assist a high-solid feed treatment efficiently.

In addition, digester shapes may govern the flow patterns, velocity, and viscosity distribution in the active volume of a digester. It also influences microbial mobility, nutrient accessibility, flow rate, and temperature [74]. Vesvikar et al. [75] compared two conical bottom digester configurations. The first bioreactor had a 25° angle and the other bioreactor had a 60° angle. The authors concluded that the lower slope angle could aid in achieving homogeneity and improve mixing efficiency in a shorter time. Similarly, Oloko-Obo et al. [76] studied the influence of biodigester shape on biogas yield. To do so, they considered a biodigester volume of 15l with three different forms (cubical, conical, and cylindrical) that operated with a substrate consisting of cow manure, poultry droppings, and hog waste under steady-state conditions. The biogas production from the cubical, cylindrical, and conical-shaped digesters began on the seventh and sixth days, respectively. The difference in the lag phase was due to the difference in time required by different microbial communities to adapt to changed environmental conditions. The maximum volume of biogas (23.4l) was produced from a cylindrical digester, whereas the conical and the cubical digesters produced 14.4 and 18.2 dm<sup>3</sup>, respectively. Furthermore, the cylindrical-shaped digester yields higher biogas production compared to other digesters. In continuous processes, employing divided digesters leads to significant increases in methane yields by facilitating proper microbial processes across different phases of anaerobic digestion. Therefore, the design of the digester should be studied alongside its operational parameters, including hydraulic retention time (HRT), temperature, organic loading rates (OLRs), substrate composition, and functional units. Figure 2 shows the innovative approaches applied to optimize and simulate the AcoD process to optimize biogas production.



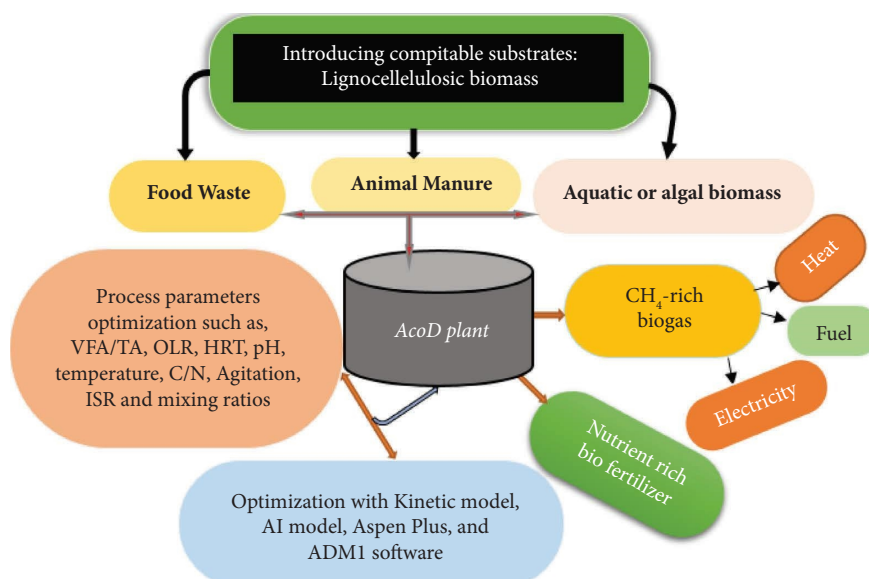


FIGURE 2: Integrating process parameters, mathematical models, and simulative tools to optimize AcoD systems and application of biogas.

#### 4. Kinetic Models and Artificial Intelligence for the AcoD System Optimization

**4.1. Models.** Table 3 summarizes the theoretical models applied for the simulation of biodegradation kinetics and their mathematical equations. The first-order kinetic model (FOKM) is a high-production-level dynamic modeling approach that considers the global response of production. Raw material digestibility is analyzed by the first-order natural calculation formulation of the batch system highlighted by Yusuf et al. [77], as shown in Table 3. This model helps to predict how the system will react to changes in mass and energy over time, as well as manage and optimize the system's performance with a different substrate introduction [82]. It can provide a reasonable fit for the exponential phase of anaerobic digestion, where the production rate is proportional to the substrate concentration. This model assumes a linear relation between reaction rate and substrate concentration. In the biogas production process, the kinetic rate can be influenced by different factors, such as temperature, substrate inhibition, pH, and microbial interactions. Nevertheless, it may not accurately reflect complicated dynamics and may also not be appropriate for systems with various constraints. In addition, it does not clearly consider the lag and stationary stages of AD, limiting its accuracy in describing the complete dynamics of the AD process.

The Cone model (CM, Table 3) is the modified Monod model (MM) that involves a factor for process inhibition at a higher substrate concentration [78]. CM fits well when there is a linear decline in biogas generation after getting a threshold point. Like FOKM, the CM does not account for the lag and exponential phases, which may limit its capability to capture the complete dynamics of the AD process. CM assumes a linear decline, which may not perfectly describe the complexities of the stationary phase. Also, it may not capture the gradients of substrate concentration, pH, and

microbial activity that are present in real biogas production systems. The Haldane model (HM, Table 3) is a more sophisticated equation with terms for both substrate inhibition and substrate limiting [79]. HM can inspect systems with many substrates and the possibility of inhibitory effects. It can fit different phases of the AD process, such as the lag, exponential, and stationary phases. However, it cannot perfectly elucidate the actual behavior in AD systems, wherein growth rates of microbial groups can be more complex, involving manifold limiting factors, inhibitions, and interactions. The MM (Table 3) is a commonly applied model in biogas kinetic simulations due to its simplicity [78]. MM accounts for substrate limitation, which is often detected in the exponential phase of the AD process and often used to characterize microbial growth in response to substrate concentration. However, the MM does not clearly reflect the lag and stationary phases of the AD system, limiting its accuracy in apprehending the complete dynamics of the process. The Weibull model (WM, Table 3) is flexible and can fit a varied range of biogas production phases, including lag, exponential, and stationary phases [80]. It can represent the nonlinear reduction in biogas production rate, which may better reflect the dynamics of the stationary phase. However, this model assumes a specific shape parameter that determines the biogas production rate decay. In practice, various factors, such as changes in substrate composition, pH, and temperature, can affect biogas production, and these factors may not be accurately represented by a single shape parameter. The transference function model (TFM, Table 3) is a linear model that describes the input and output parameters based on transfer functions, providing a more detailed kinetics of the biogas production process. It can fit different stages of the biogas production process (lag, exponential, and stationary phases) [81]. While this model can provide insights into the dynamic behavior of the AD process, it may not fully capture the nonlinearity and complexities related to substrate



TABLE 3: Kinetic models of cumulative gas production.

Models	Equations	Parameter description
First order [77]	$M = M_o [1 - \exp(-k_i * t)]$	$M$ = cumulative methane produced (ml/gVS)
Cone [78]	$M = M_o / (1 + (k * t)^{-n})$	$M_o$ = methane predicted (ml/gVS)
Haldane [79]	$M = M_o * (C / (k_c + C) (1 + C / k_i))$	$k_h$ (d) = hydrolysis rate constant
Monod [78]	$M = M_o * (k * t / (1 + k * t))$	$C$ = VS ratio of a cosubstrate over the total substrate VS (%)
Weibull [80]	$M = M_o * (1 - \exp(-k * (\lambda - t)^n))$	$K_c$ = the half-saturation constant of cosubstrate (%)
Transference [81]	$M = M_o \{1 - \exp[-R_m / M_o (t - \lambda)]\}$	$K_i$ = half inhibition constant of the cosubstrate (%)
Modified Gompertz [78]	$M = M_o \exp\{-\exp[R_m * e / M_o (\lambda - t) + 1]\}$	$\lambda$ = phase delay time
Modified logistic [81]	$M = M_o / 1 + \exp[4R_m / B_o (\lambda - t) + 2]$	$R_m$ = maximum biogas production rate (ml/gVS.d)
Modified Richards [81]	$M = M_o [1 + \exp\{R_m / M_o (1 + 1/n) (\lambda - t)\}]^{(-1/n)}$	$n$ = shape factor, $k$ = rate constant (1/d), $t$ = digestion time (d), $e = 2.718$

degradation, microbial growth, and biogas production rates. For example, Robert et al. [78] analyzed the kinetics of the codigestion of rendering industry and food wastes in two-phase anaerobic digestion. They identified that the first-order kinetic model effectively matched the experimental data with an increment of kinetic reaction constant from 0.135/d to 0.150/d. Another study evaluated the effects of inoculum types on  $\text{CH}_4$  yield in the codigestion of primary sewage sludge and hydrothermally treated waste-activated sludge through experimental and kinetic methods (Cone, modified Gompertz, Gompertz, first-order, and Weibull models) under mesophilic conditions. The results showed that except for MGM, all models describe the evolution of gas production well for both inoculums, with high correlation ( $R^2 > 0.976$ ), as shown in Table 4. In addition, Zhen et al. [87] combined food waste and microalgae to evaluate synergistic effects through experimental and kinetic studies (i.e., FOKM, MGM, and CM) at different mixing ratios. CM had the best fitness to the experimental data and could elucidate the codigestion process kinetics more sensibly ( $R^2 > 0.963$ ).

**4.2. Bacterial Growth Curve Models.** Several sigmoidal functions (Gompertz, logistic, and Richards) are developed to describe a bacterial growth curve under different physicochemical conditions. These models allow the estimation of microbial safety, the detection of critical points of the production and distribution process, and production optimization. Unlike the FOKM, the modified Gompertz (MGM), logistic function model (LFM), and Richards (MRM) models predict the cumulative methane production rate and lag-phase time, a crucial indicator reflecting the productivity of the biogas production process. Table 3 represents the modified Gompertz and logistic function models, respectively [88].

The MGM and LFM are the most commonly used models to find the biogas kinetic parameters as they fit the three stages of biodegradation processes: the lag, exponential, and stationary phases with a high degree and accuracy. The MGM and LFM were more often utilized than the first-order model since they were connected with two biological reaction parameters,  $R_m$  and  $\lambda$  (Table 3). Furthermore, both models provide details about the exponential curve associated with the exponential bacteriological growth. Both models seem to be similar. The main difference between them is that the curve of MGM is symmetrical, whereas the LFM is asymmetrical [89]. However, the intrinsic shortcoming of both models is that when used to represent biogas production (Table 3), neither achieves the initial condition ( $M = 0$  at  $t = 0$ ) [90] unless the parameter approaches infinity for MGM. Both models have been developed to depict bacterial and biological growth rather than biogas production, because the two scenarios had different initial conditions [88]. In addition, these models explain only the quantity of microorganisms but do not include the substrate consumption as a model based on the Monod function would do [88]. In the case of methane production from wastewater, the initial microbial mass is not zero due to the

input of anaerobic-activated sludge seeds to the bioreactor (Table 3 is different from at  $t = 0$ ), although the gas volume (methane) is zero. In addition, another issue with the MGM for product generation is that the lag time fitted from experimental data is occasionally negative, which occurs when products are formed nearly instantly without lag day. The gas is formed quickly during wastewater AD that is fermented with acclimatized anaerobic sludge. Thus, it is important to develop emerging models that simulate substrate consumption, microbial growth, and biogas production [90]. The Richards model (Table 3) is commonly used to describe the growth and activities of microbiological systems. It is adept at capturing a wide range of growth patterns, including sigmoidal and nonsigmoidal stages [88]. This flexibility suits it to possibly fit the different phases of biogas production, including lag, exponential, and stationary stages. Similar to the MGM and MLM, the parameters in the Richards equation often have clear biological interpretations [81]. For example, the maximum growth rate and lag time can be related to microbial activity and substrate availability. It is a generalization of the logistic model, and it presents four parameters, including a curve shape coefficient [81]. The model's flexibility makes it a valuable tool, but the limitations associated with parameter estimation challenges, model complexity, and interpretation might be considered when applying the Richards model to biogas production process simulations. In addition, like modified Gompertz and logistic models, the MRM may be sensitive to the initial condition estimates [88], leading to potential difficulties in accomplishing reliable parameter estimation. For example, Ali et al. applied the Gompertz, logistic, and Richard models for the modeling of the cumulative biogas production kinetics. The result showed that the Richards model best fits the experimental data with the lowest error value (RMSE = 1.077) for cow manures, among other sinusoidal growth function models, while the first-order model exhibited the maximum difference between the actual and predicted data (11–43%) [85]. In another work, Yu et al. [84] compared four biogas kinetic models (FOKM, LFM, CM, and MGM) to evaluate the biokinetics of biogas production from wheat straw (WS), sugarcane bagasse (SB), and rice straw (RS) codigestions. The overall kinetic parameters dictate the LFM to reproduce the experimental results with higher accuracy, followed by the MGM. The selection of the model is determined by the specific characteristics of the system, available data, and the research objectives. Thus, it is important to calibrate and validate the selected model using experimentally measured data from the specific AcoD process of interest to ensure its reliability in prediction. A brief overview of the models and their typical applications are shown in Table 4.

In Section 4.2, the benefits and limitations of different models in simulating biogas production kinetics, considering their fitness for each stage, were summarized. In terms of reliability for biogas simulation and optimization in the AcoD process, there is no one-size-fits-all answer. In real cases, the reaction kinetics can be biased by different factors such as substrate availability, temperature, pH, and microbial interactions. However, some of them assume

TABLE 4: Summary of the achievements with kinetic models.

Models	Cosubstrates	Achievements	Ref.
MGM and FOKM	Water hyacinth and food waste	The models give maximum biogas production, reaction kinetics, and production delay phase under different conditions, depending on the ultimate biogas production curve. Codigestion kinetics estimated and well fitted by MGM with a minimum deviation of 2.84–13.01%	[21]
FOKM and TFM	<i>R. Okamura</i> and OMSW	The model is applied to assess the biokinetic parameters (hydrolysis kinetics, maximum biogas production, and maximum biogas production rate). The best kinetic results of the AD process were obtained by both models	[22]
FOKM and MM	Food waste and rendering industry streams	The models give biokinetic parameters and maximum biogas production. The best fit to experimental data was obtained by the FOKM with high correlations	[78]
MGM, FOKM, CM, and WM	Sewage sludge and treated waste-activated sludge	The models described the evolution of gas production and reaction kinetics. Models described lag, exponential, and stationary phases. Except for MGM, all functions interpreted the gas production evolution well ( $R^2 > 0.976$ )	[80]
FOKM, CM, MGM, and TFM	Chicken litter (CL) with yogurt whey (YW), hay grass (HG), and wheat straw (WS)	The model explains optimum mixing ratios and gives maximum CH <sub>4</sub> production rate and lag-phase time with reliable fitness. For all tests, the MGM was the best fit for measured data with $R^2 > 0.931$ and deviations between measured and predicted one as <9.93%	[83]
MGM, CM, FOKM, and MLM	Corn stover (CS) and chicken manure	The model simulated biogas production, maximum biogas production rate, hydrolysis rate, and lag stage under various conditions with the best accuracy. Among these models, MGM was the best fitted in elucidating the methane production process ( $R^2 = 0.984–0.998$ )	[84]
FOKM, MGM, and MRM	Cow and sheep manure	The model computes the potential biogas production, the maximum biogas production, and the production delay time under different conditions based on the ultimate production curve of yield. MRM best fitted to experimental data with high correlation $R^2 > 0.981$ and lower RMSE value = 0.589 for sheep manure	[85]
MLM, MGM, and TFM	Yard waste and food waste	The models gave maximum gas production and evaluated the biokinetic parameters by nonlinear regression analysis. The lowest difference between experimental data and predicted data was observed in MGM (3.7–15.4%), followed by MLM (4.9–18.9%). The statistical indicators ( $R^2$ and RMSE) reflected the best fitness of MGM to experimental data with the highest $R^2$ (0.994–0.996) and lowest RMSE (3.7–15.4)	[86]

RMSE, root mean square error;  $R^2$ , correlation coefficient.

a constant kinetic rate throughout the process, which may not precisely represent the complex biogas production dynamics. In addition, the relationships between specific microbiological processes and kinetic parameters may not always be forthright or easily discernible. Thus, the kinetic model does not sufficiently capture the interactions and competition between different microbes or the influences of multiple substrates on the AcoD performances. Besides, it is essential to develop novel models, which properly describe the AcoD process for real applications.

#### 4.3. Role of Artificial Intelligence (AI) in AcoD Processes.

The AcoD has several advantages over mono anaerobic digestion, including improved biodegradation and system stability, which in turn boost the biogas production and methane yield. An efficient AcoD performance requires a full understanding of the effect of process parameters and the kinetics of biodegradation. The actual process control and optimization could not be achieved without predicting the performance of the system precisely [91]. So far, various hypothetical and mechanistic models have been developed to control and monitor the AcoD process, elucidate process inhibition, and optimize biogas production. However, such traditional approaches not only require prior knowledge but also are complex, laborious, and depend on very few scenarios. Thus, AI-based algorithms are found to be suitable for capturing the complex and nonlinear nature of AcoD processes, which could not be achieved mechanistically [92]. They have made the nonlinear, mathematically complex, laborious, and time-consuming AcoD process quite easy and manageable. In the subsequent subsections, the role of ANN, GA, and hybrid models are discussed concerning the AcoD process controlling, monitoring, and biogas production optimization [93].

**4.3.1. ANN Models.** ANN models have been developed to predict the yield, rate, energy content, and composition of biogas produced from different types of inputs. In this case, the experimental data arrangements need to be divided into three different sets: training, testing, and validation datasets. ANNs can take in multiple inputs and process them to produce single or multiple outputs [93]. The accuracy of the developed ANN models is measured using statistical measures, such as the mean absolute deviation (MAD), mean square error (MSE), RMSE [94], and  $R^2$  [95]. ANN models are used to model the behavior of different linear and nonlinear processes with higher accuracy. ANN is the most recent and popular model used to simulate the complex AcoD processes and parameters and to predict biogas production and the composition of biogas produced. The effectiveness of an ANN model in predicting biogas production depends on the quality and quantity of data used for its training. The ANN models may predict biogas production,  $H_2S$ , and  $NH_3$  traces [93] based on several input parameters, such as feed type, soluble COD, pH, HRT, OLRs, C/N, and mixing ratios (Table 5). Several researchers have developed ANN models to predict biogas production. For instance, Kola et al. [94] used process parameters such as

total dissolved solids (TDS), pH, mass of the slurry, temperature, dissolved oxygen (DO), and BOD as input parameters to model biogas production from the codigestion of cattle dung and poultry droppings using MATLAB R2015 tool. Similarly, Wang et al. [95] developed an ANN-based model for monitoring alkalinity online from the codigestion of maize straw, fruit, and vegetable wastes with cow dung. The researchers inserted electrical conductivity, redox potential (ORP), oxidation, and pH as input parameters with the soft sensor method based on ANN. They demonstrated the reliability of the developed ANN model through sensitivity and accuracy analyses. In another study, Seo et al. [101] integrated a process-based approach with a recurrent neural network black-box model to forecast biogas production and organic loading rates from AD of food waste. The results show that the developed model precisely estimated the biogas production rate with inputs as soluble COD, retention time, and VFA. Figure 3 illustrates the simple neural network architecture with three layers (multiple input, hidden layers, and output) to predict products.

Some researchers achieved remarkable outcomes when neural network techniques were integrated with fuzzy-logic approaches, sometimes known as neuroadaptive fuzzy logic. The adaptive network-based fuzzy inference system (ANFIS) algorithm is a class of ANNs that solve problems related to functional approximation. For example, Najafi and Ardabili digested spent mushroom compost (SMC) and modeled the experimental data to determine the biogas yield at mesophilic and thermophilic temperatures using ANFIS, ANN, and logistic models for comparison. The statistical references such as RMSE and  $R^2$  were reported to be 0.1940 and 0.9998 for the ANFIS network, 0.780 and 0.9981 for the multilayer perceptron (MLP) network, and 0.5111 and 0.9992 for the logistic model at a mesophilic temperature of 35°C. Similarly, the RMSE and  $R^2$  values were reported to be 0.3033 and 0.9997 for the ANFIS network, 0.3430, and 0.9992 for the MLP network, and 0.5506 and 0.9991 for the logistics model, respectively, at a thermophilic temperature of 55°C. Based on a comparative analysis using the RMSE and  $R^2$  values as a standard for comparison, it was determined that the ANFIS network yielded more accurate and dependable biogas yield predictions at both mesophilic and thermophilic temperatures [24]. In another study, Rafiee et al. [103] applied ANN and ANFIS models to estimate biogas production from wastewater treatment at a laboratory scale in an anaerobic reactor. The results revealed that the two models successfully predicted biogas production with high accuracy. An overview of other related literature reveals that the ANN model is an influential tool for simulating and forecasting the influences of various process parameters and substrate composition on biogas production (Table 5). However, the application of ANNs in modeling AcoD systems is hindered by challenges such as poor generalization (the ANN models' ability to adapt to previously unseen data) and a limited dataset of standalone ANN models. In addition, the black-box nature of multiple-layer models and the lack of interpretability of developed ANN models when applied to the design, simulation, and

TABLE 5: Summary of the application of the AI approach in biogas prediction.

AI type	Objectives	Input parameters	Optimum models	Output	Ref.
ANN	To develop a model to forecast the effects of process parameters	COD, BOD, flow rate, recirculated sludge flow, and feed rate	ANN-MLP	Biogas yield	[96]
ANN	To develop a numerical simulation model to estimate the optimum biogas production	Feed type, volatile solid (VS), pH, OLR, HRT, temperature, and reactor volume		Cumulative biogas yield	[97]
ANFIS and ANN	To estimate the biogas yield	C/N ratio, reactor temperature, and RT	ANFIS	Biogas	[24]
ANN	To simulate and model the performances of the codigestion process	Mix ratios and RT	ANN-Bayesian regularization algorithm	Methane yield	[98]
ANN	To model the relationship among the physicochemical parameters of a blend of codigestion of cattle dung and poultry droppings to estimate biogas production	Mix ratios, pH, TDS, temperature, slurry, BOD, and DO		The volume of biogas yield	[94]
ANN-GA and ACO	An integrated model to predict and evaluate the biogas production rate	TSs, VSs, acid detergent fiber, acid detergent lignin, NH <sub>3</sub> -N, VFA, HRT, and OLR	ANN with GA and ACO	Biogas production rate	[99]
ANN-GA	Optimization and prediction of the amount of biogas generation from codigestion of selected substrates	pH, C/N ratios, and SRT	ANN optimized with GA	Biogas generation	[92]
ANN-GA	To model and optimize mixing ratios in the codigestion process	Substrate-to-inoculum ratios, mix ratios, temperature, SRT, and feed type	ANN-GA	CH <sub>4</sub> production	[100]
RNN	To estimate the biogas production rate	SRT, soluble COD, total VFA, free ammonia, and total ammonia		Biogas production rate	[101]
ANN-PSO	To optimize and forecast the biogas generation from codigestion of cattle manure (CM) and palm oil mill effluent (POME)	Mixture ratio, oxidation by hydrogen peroxide, and ammonium bicarbonate		Biogas yields	[102]

RNN, recurrent neural network; SRT, solid retention time.

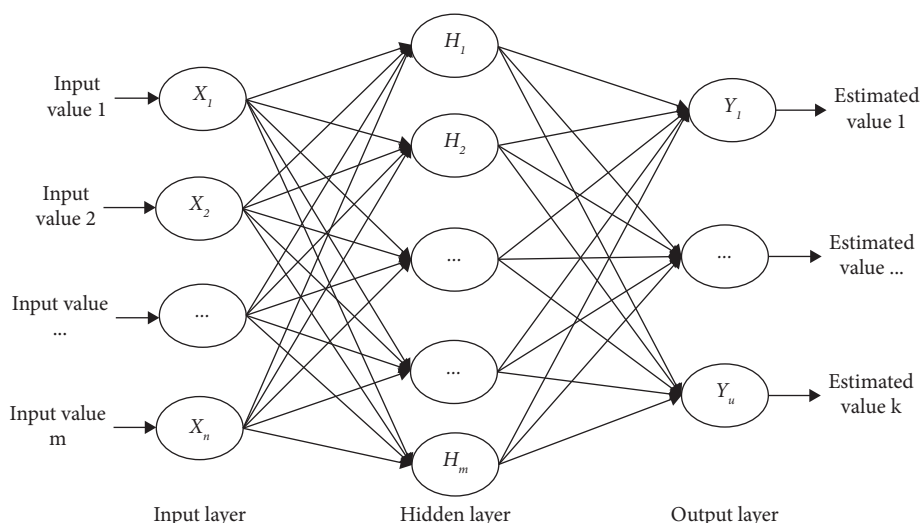


FIGURE 3: Simple artificial neural network architecture (adapted with permission from [82]).

optimization of AcoD processes for enhancing biogas production are challenging. This lack of interpretability makes it difficult to gain insights into the specific factors influencing biogas production or to detect potential points for process enhancement [23]. Another limitation of the ANN model is the requirement for large and representative datasets. The ANN model requires a substantial amount of data to be trained efficiently and accurately in order to demonstrate the underlying configurations and relationships. In the case of the AcoD process, acquiring wide-ranging and high-quality datasets may be challenging due to the inherent inconsistency in substrate composition, environmental conditions, and digester performance [93]. Furthermore, whether the dataset is small or the model is extremely sophisticated, ANN models are prone to overfitting, as they are based on training data and often fail to generalize to previously unseen data. Consequently, this can lead to poor performance when using the trained ANN model to simulate or optimize various operating parameters in the AcoD process [95]. To address these challenges, it is critical to carefully preprocess and refine the dataset, ensure data representativeness, and routinely check the ANN tool against independent experimental data. Furthermore, hybridizing the ANN model with other approaches and methodologies, such as mechanistic models or optimization algorithms, may give a comprehensive and reliable method for modeling AcoD processes to monitor, control, and optimize biogas production.

**4.3.2. Genetic Algorithm.** From the viewpoint of AI research, the learning mechanism offered by GA is noteworthy. The typical strategies employed in all GAs are inheritance and birth traits, mutation and change to prevent resemblance, natural selection, and variation to improve longevity and crossover. The GA is an effective domain-independent search method based on biological principles [93]. GAs offer several benefits, making them a common option for the optimization of biogas production in AcoD systems. The advantage of GAs is that they use a population-based

approach rather than a single solution. This approach helps protect the algorithm from getting stuck in suboptimal solutions and promotes the detection of several potential solutions [93]. The objective function of GAs may exhibit multiple troughs or peaks, rendering them highly effective in addressing nonlinear and multimodal optimization problems. In addition, GAs can be applied to optimization problems where the underlying system is treated as a black box, requiring no detailed knowledge of its internal workings. This characteristic makes GAs suitable for real-world applications in which the system's behavior may be complex or not fully understood [104]. Despite these benefits, GAs have some limitations in the context of predicting biogas production, such as dynamic changes in substrate composition, microbial populations, and environmental conditions associated with AcoD. GAs involve the evaluation and iteration of multiple candidate solutions, which makes the procedure computationally intensive, especially when dealing with large datasets. GAs may face challenges in adapting rapidly to dynamic changes, and their static nature may not capture the embryonic nature of the biogas production process [23]. GAs often requires problem-specific tuning to attain optimal results, which can make them less user-friendly for practitioners lacking expertise in algorithm parameterization [105]. However, the algorithm's performance can be affected by the selection of initial parameters, and identifying an optimal parameter set may entail additional computational effort [104]. In addition, the effectiveness of GAs can be affected by how the problem is represented, such as the encoding of parameters and the selection of a specific genetic operator. Integrating GAs with other optimizing models may help mitigate some of these challenges [106]. Table 5 shows the different achievements with GA tools.

**4.3.3. Hybrid Models.** Integrating an ANN with evolutionary algorithms predicts and optimizes various nonlinear bioprocesses. The common evolutionary algorithms include GA, ACO, and PSO [99]. These algorithms have been

hybridized with the ANN model to estimate biogas yield and percentage of methane content in the produced gas. Zaied et al. [102] integrated ANN with PSO to simulate the AcoD process in a solar-aided biodigester. The researchers confirmed that the proposed model was flexible and effective in forecasting biogas production. Similarly, Beltramo et al. [107] coupled the ANN with optimized ACO to predict biogas production. They revealed that the hybrid model provided a reliable approach to analyzing the AcoD process. In another study, Beltramo et al. [99] simulated the biogas production process and predicted the biogas production rate by integrating ANN, GA, and ACO models. ACO and GA were employed to select variables. As input parameters, they used volatile fatty acids, volatile solids, acid detergent fiber, total solids, acid detergent lignin, neutral detergent fiber, ammonium nitrogen, hydraulic retention time (HRT), and organic loading rate (OLR). These researchers confirmed that the model dimension reduction enhanced the capacity of ANN models to forecast biogas production rates, as indicated by  $R^2$ .

## 5. Modeling and Optimization of AcoD Process

The difference between modeling using kinetic models and software, such as AP and ADM1, lies primarily in the level of detail, the complexity of the models, and the flexibility and computational capabilities of the software. While kinetic models focus on the detailed representation of reaction kinetics in specific systems, AP and ADM1 offer a broader scope for modeling complex biochemical processes, including AcoD processes, while considering a wide range of factors beyond kinetics. This software allows one to simulate and analyze complex biochemical processes involving multiple unit operations, fluid flow, heat and mass transfer, and phase equilibria. AP and ADM1 models also provide a more user-friendly interface, extensive libraries of prebuilt models, and computational capabilities for comprehensive process simulation and analysis, making them suitable for process design, optimization, and scale-up studies. Optimizing a variety of AcoD process parameters with objectives such as maximizing biogas production, reducing energy consumption, and avoiding environmental impacts can be carried out using different modeling and simulation tools. In this work, the role of AP and ADM1 models in the simulation and optimization of the AcoD process, as well as their limitations and advantages, is discussed in the following sections.

**5.1. Aspen Plus (AP).** Understanding different factors in a controlled condition is important to form a proper environment for anaerobic microorganisms to function properly for the desired biogas production [20]. The chemical contents and biodegradability of substrates may vary to classify and predict the system, but they are the fundamental issue in modeling the AcoD process correctly [108]. Moreover, experimental techniques may occasionally be costly and time-consuming, and outputs might be incorrect; therefore, process simulations are essential.

However, an inadequate simulation method might give inaccurate results if proper assumptions are not used. Therefore, more research efforts should be made to identify the best simulation models that may optimize the AcoD process to enhance biogas production. This reduces time and excessive resource usage. Several researchers have used different models to simulate the AD process reaction paths, including AP [109, 110], ADM1 [111, 112], and Design-Expert software [113]. AP is a comprehensive process simulation tool that can be applied to a broad range of biochemical processes, which makes it suitable for several applications beyond AD. It has many benefits, including allowing a selection of prebuilt models for immediate use, such as pumps, compressors, mixers, separators, reactors, heat exchangers, and the like. This model can also be improved by using optional add-on applications such as Aspen Plus Dynamic, Aspen Energy Analyzer, Aspen Custom Modeler [114], and so on. In addition, with the world's largest property database and exceptional flexibility in handling solid, fluid, and gas phase processes, AP offers the option of using other programming software, such as Excel, FORTRAN, Visual Basic, and MATLAB, to expand the Aspen features. It also facilitates the construction of expansive flow-sheets by incrementally adding a few blocks at a time. Built-in features activated economic tool that provides access to information about capital and operational costs from the flowsheet [115].

The AP reactor models include the stoichiometric reactor, the CSTR, and the RYield reactor, which are used as reaction environments in the different phases of AD reactions [20]. The simplest schematic diagram for simulating an AcoD process using Aspen Plus is depicted in Figure 4. Aspen Plus incorporates various thermodynamic models to represent the physical properties of components and mixtures within the process. Since they can accurately depict the behavior of the nonideal mixtures, the activity coefficient models of Wilson, nonrandom two-liquid theory (NRTL), and universal quasi-chemical theory (UNIQUAC) are among the most commonly used thermodynamic models for the study of a significant number of binary and multi-component systems. The original NRTL, electrolyte NRTL (e-NRTL), polymer NRTL, and segment-based NRTL (NRTL-SAC) are some of the various versions of the NRTL models [117]. NRTL offers more flexibility in the phase equilibria description than other thermodynamic models owing to the additional nonrandomness parameters. For AD process simulation, several researchers selected the NRTL model as the property method since the reaction concerned liquid and gas phases to calculate mole fractions and activity coefficients [19, 20, 118]. For example, Inayat et al. [118] developed the simplest model to design and simulate the AcoD system in Aspen Plus 7.3.2 using the NRTL as the property method to notice the best combination that maximizes the biomethane in biogas. To achieve their objectives, stoichiometric reactors and CSTRs were used for the hydrolysis stages, while for the remaining three stages, existing reactors in the AP software were employed. In AP software, sensitivity analysis, regression plot, and confidence interval were used to assess the model's fitness with the



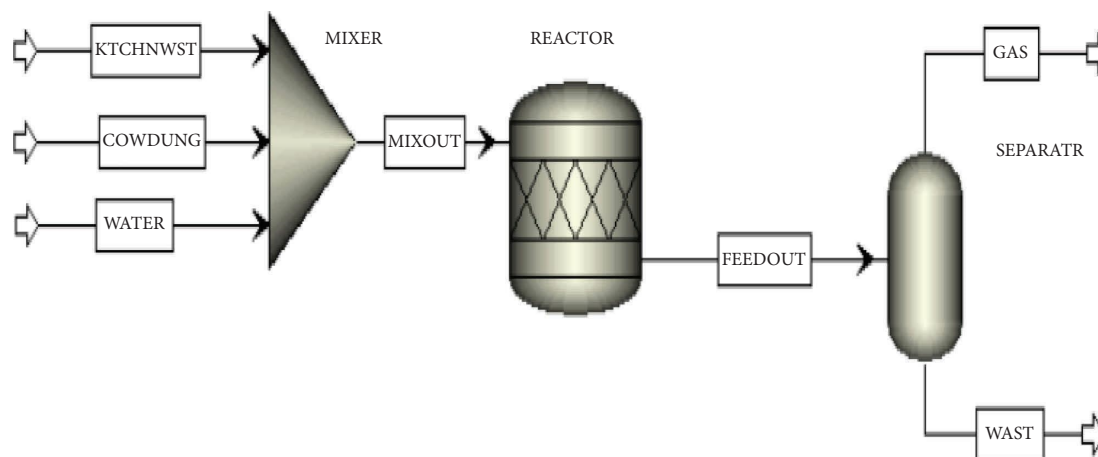


FIGURE 4: AcoD process simulation flowsheet using Aspen Plus software adapted with permission from [116].

experimental results. In addition, differences between the experimental data and process simulation results were calculated using sensitivity analysis [119]. However, notwithstanding the flexibility to reproduce, the complicated behaviors of the aforementioned NRTL models are correlative, which limits their application since experimental data to regress the NRTL interaction parameters are required. In addition, the Soave–Redlich–Kwong (SRK) and Peng–Robinson (PR) equations are the most commonly used in Aspen Plus. These equations have been successfully applied in various industrial biogas production processes. These equations can handle complex vapor–liquid and liquid–liquid equilibria, making them suitable for simulating the phase behavior of various biogas components such as methane, carbon dioxide, and trace impurities. The selection between the SRK and PR equations depends on the specific characteristics of the system and the available experimental data for model parameter estimation. Generally, the PR equation is more accurate than the SRK for systems containing polar or associating components. However, the SRK equation is computationally less intensive and can be more efficient for simulating simple gas mixtures.

The AP process simulation model was developed mainly based on the different steps of the AD process, including hydrolysis, acidogenesis, acetogenesis, and methanogenesis [19]. These four stages describe just how the complex organic substrates can be broken down into their monomers and finally into biogas rich in  $\text{CH}_4$  and  $\text{CO}_2$ . The AD process simulation flowsheet was constructed based on the experimental results. Despite these advantages, the widespread adoption of AP software for modeling and optimizing the reaction process in AcoD reactors has been limited. There is a scarcity of research articles available on AcoD simulation and optimization using AP. However, AP simulation approaches have recently been employed for simulating the AcoD reaction process. Martínez-Ruano et al. [114] modeled the AcoD of potato stem and milk whey using the stoichiometry approach and kinetic models in AP, aiming at simulating biogas production, technoeconomic feasibility, and heat and electricity generation. They concluded that the setups operated with a high organic load were best in terms

of biogas generation and economic evaluation. Their results also show the dominant influence of raw material cost compared to the total cost of biogas processing (~80%). In another experiment, Oladiran and Columbro [116] simulated the AcoD process using the stoichiometry method and an operating condition of  $25^\circ\text{C}$ ; the degradation reaction involved carbohydrates and proteins since their mass composition is necessary to perform the simulation. However, fats are not included due to the absence of  $\text{CH}_4$  or  $\text{CO}_2$  in the products. Similarly, Inayat et al. [118] simulated the AcoD of animal byproducts and wastewater as main substrates using Aspen Plus. They compared the results of five groups of cosubstrates at various ratios to observe the contents of  $\text{CO}_2$  and  $\text{CH}_4$  in the biogas. The results revealed that the codigestion data of tree leaves, animal manure, and wastewater at 25:25:50% produced a maximum methane yield of 50.55 mol%. In the same experiment, the mixed seeds, animal manure, and wastewater at 25:25:50% resulted in the highest  $\text{CH}_4$  yield of 47.85 mol% with low emission, which is more attractive and recommended. In addition, Janošovský et al. [120] used AP to simulate and optimize the process and economic benefits of biogas generation for the dairy plant. Process parameters, such as biogas price after desulfurization, methane content, fresh milk, and milk powder prices, were used in the parametric sensitivity analysis. They evaluated various effects of biogas use depending on biogas treatment costs, market prices, and methane content. The authors demonstrated that the injection of biogas into boiler fuel reduced the payback cycle from 11.2 to 5.1 years. Furthermore, Capra et al. [121] developed a multiobjective optimization model to identify the trade-off between capital cost and energy consumption during a biogas upgrade to  $\text{CH}_4$  using AP software. The results showed that the capital cost decreased by 17%, while the energy consumption increased by 27%. Table 6 summarizes some of the biogas simulation results using AP. However, there are some challenges associated with using AP in the design and optimization of AcoD process parameters: AcoD system involves complex chemical reactions. Modeling these details precisely in AP can be challenging, especially when dealing with the nonideal

TABLE 6: Summary of Aspen Plus and ADM1-based biogas simulation and optimization models.

Model	Mono/cosubstrates	Objectives	References
AP	Wastewater	To simulate and optimize the operating parameters, including OLR, temperature, effects of H <sub>2</sub> addition/pH value, and recycle ratios to maximize biogas production	[122]
	Waste sludge and expired yogurt	Prediction of kinetic parameters and simulation of codigestion	[112]
	Cattle manure and dairy milk processing waste	To simulate dairy milk process plant and investment profitability of biogas use in drying milk	[120]
	Cow dung and food waste	To simulate codigestion to predict the amount of biogas production	[116]
	Potato stem and milk whey	Optimization of organic load and evaluation of technoeconomic assessment	[114]
	Pulp mill primary and secondary sludge	To evaluate the potential of bioenergy production and optimization of mixing ratios	[123]
	VOC emissions	To optimize and simulate biogas production	[124]
	Palm oil mill effluent	To optimize process parameters to produce maximum methane	[125]
	Cow manure	Modeling and optimization of biogas and hydrogen production and effects of process parameters	[126]
	Municipal solid waste	To optimize and analyze methane production	[127]
ADM1	Food waste and primary sludge	To model biogas production, combined heat and power, economic analysis, and optimization of mixing ratios	[128]
	Food waste	Effect of hydraulic retention time (HRT), C/N ratio, and changes in feed composition on the biogas production	[129]
	Municipal solid waste	To optimize and simulate the OLRs, pH, and other parameters	[111]
	Solid waste	To investigate the effects of pH and VFA on biogas production	[130]
	Primary sludge	To simulate the dynamic properties of a primary sludge digester in a full-scale digester	[131]
	Pig manure with silages, thin stillage, and glycerine phase	To optimize and simulate codigestion and kinetic parameters to predict biogas production	[132]
	Lactate	To assess the effect of adding lactic acid into ADM1 in influencing the prediction potential of the model	[133]
	Food waste and waste-activated sludge	To model, predict, and simulate operational performances and biological behavior of monodigestion/codigestion	[134]
	Dairy manure spent and mushroom substrate	To model and predict pH and the kinetics of biogas production to optimize the substrate ratio and HRT	[135]
	Waste-activated sludge and corn silage	To simulate and optimize the mixing ratio to achieve maximum methane production	[136]
ADM1-PID	Diluted dairy manure kitchen wastes	To optimize the mixing ratio of codigestion and HRT and to evaluate hydrolysis kinetics to enhance methane production	[137]

behavior of components [118]. In addition, finding reliable models for the AcoD process components can be difficult, leading to uncertainties in the simulation results. AP requires reliable input data such as physical-chemical properties, reaction kinetics, and thermodynamic parameters for the AcoD process components [114]. Attaining accurate data for all the components involved in the AcoD system may be a daunting task, especially for novel processes. Validating the AP model for the AcoD system against experimental results is vital. However, it may be challenging due to the limited availability of data. Overcoming these limitations may require an integration of advanced modeling methods and experimental validation.

**5.2. Anaerobic Digestion Model No. 1 (ADM1).** The importance of mathematical models has become a standard tool in biogas plant design, operational control, prediction, and optimization. Although different models have been developed to predict and control the anaerobic digestion process, ADM1 was developed by the IWA group for wastewater treatment [108]. ADM1 is a structured model with biochemical processes (disintegration, hydrolysis, acidogenic, acetogenic, and methanogenic) and physico-chemical processes (liquid-gas processes and liquid-liquid processes) [82]. ADM1 becomes a powerful tool to predict and control the optimization of mono/codigestion for biogas production. It simulates constant volume and completely mixed processes, which are difficult to obtain in many AD processes, especially with large-scale plants [82]. Bułkowska et al. [132] simulated the mesophilic codigestion of pig manure, thin stillage, and glycerine phase with silages. ADM1 was extended to include the slowly and rapidly degradable portions of proteins and carbohydrates. They revealed that the developed model is less sensitive to changes in kinetic constant for rapidly disintegrated carbohydrates than to changes in kinetic constant for slowly degraded carbohydrates. The ADM1 showed good agreement with the measured daily biogas production and the concentrations of individual VFAs in the effluent after calibrating the parameters using a mixture of thin stillage pig manure and silages. Similarly, Weinrich and Nelles [138] developed a simplified four-step mass-based ADM1 model to describe detailed intermediate reaction characteristics and degradation pathways to predict biogas production potential and rate. However, it is important to integrate ADM1 with other simulative software to optimize the AcoD reaction process. Nguyen incorporated ADM1 with AP to model and simulate an AD process of food waste. The ADM1 model was modified to indicate the inhibition of acetoclastic methanogenesis by ammonia and includes a “metabolic switch” model based on the availability of key trace components to operate. The energy model, ADM1, is linked to the combined heat and power generation, mechanical processes for biogas upgrading, and digester mixing system developed in the AP simulating platform. They demonstrated that incorporating components of the software allows the accurate design of the combined heat and power (CHP) and direct heating units for a biogas plant [115]. Several researchers

simulated biogas production processes from different substrates, both for laboratory and industrial-scale biogas plants, by modifying the process parameters and reaction rates in the original ADM1 model. Zhou et al. [136] developed ADM1 with a proportional-integral-derivative (PID) controller to manage feed, simulate, and optimize the corn silage and waste-activated sludge codigestion under mesophilic temperatures. They revealed that VFA, methane production, and pH simulation correlated well with experimental data. In the same vein, Wu et al. [139] developed a modified model based on the structural modification of the original ADM1, and the developed model accurately forecasted methane production under different operating modes.

Besides, ADM1xp is one of the modified ADM1 and is more applicable for real-scale biogas plants [108]. The ADM1xp assumes a low rate of disintegration and high hydrolysis constants for carbohydrates, proteins, and lipids. One of the most important processes in the ADM1xp model is the decay of biomass, which is responsible for producing particulate organic matter. Satpathy et al. [133] extended ADM1 to include a crucial metabolic product, lactate during sugar fermentation to test the soundness of the modified ADM1 in the standard biogas reactor predictions in the batch and continuous modes. The ADM1xp model provided a positive correlation with the measured data for both tests. They justified that the inclusion of lactate in the modified model resulted in optimized simulation for biogas and % CH<sub>4</sub> in the standard reactor. According to Katarzyna et al. [140], the model calibration demonstrated that the disintegration kinetics were low, which was 0.1/d and substantially slower than the initial value in ADM1. They employed MATLAB (MathWorks, USA) as a simulative tool with the GA optimization procedure and SIMBA 6.6 software package. Typically, the ADM1xp model calibrates ammonia and hydrogen inhibitions for acetoclastic methanogenesis and acetogenesis. The ADM1xp was a more improved one than the original ADM1 model because the maximum growth rates, decay rates, and inhibition constants depended on temperature. Despite this, the ADM1xp is also complex compared to the old ADM1 model, especially when one considers the population data of microorganisms in the AcoD apart from a large number of independent and dependent variables. The ADM1 model and its revised version are unable to differentiate the varying performance levels of microbes within the same process. In the AD process, the majority of biochemical and methanogenic reactions exhibit a low exchange of Gibbs-free energy ( $\Delta G \sim 0$ ), primarily due to the absence of robust external electron acceptors. This exchange of low energy makes some key reactions during anaerobic digestion close to thermodynamic equilibria [108]. The dynamic equilibrium model indicates that the biochemical processes occur near the equilibria and it would involve the development of bio-kinetic models of the AcoD process [115]. The decomposition of biomass, which leads to the production of particulate organic matter, is among the crucial processes that require modeling in ADM1. However, dynamic modeling overlooks the system's thermodynamic properties and

challenges related to optimization and stability in the digestive system remain unresolved. Therefore, it is essential to incorporate dynamic modeling that considers the thermodynamic characteristics of the codigestion process. By understanding the thermodynamic characteristics, specifically the activity coefficient, of codigestion processes and incorporating them into ADM1 modeling, it is possible to improve biogas production control mechanisms and reduce the complexity of the AcoD reaction process [108]. As a result, the model requires more research into characterization methods and parameter calibrations. Table 6 also shows some of the biogas optimizations with ADM1.

**5.3. Comparison of AP and ADM1 Models.** Comparing AP and ADM1, the ADM1 model was used the most frequently and was highly cited by several authors. However, ADM1 requires detailed input data and calibration to represent precisely a specific AcoD system. Obtaining the necessary input information and calibrating the model may be time-consuming and challenging [108]. In addition, while ADM1 may be applied for process optimization, its main purpose is not optimization out of the box. Optimization with ADM1 should typically involve setting model parameters to match actual data or preferred process performance rather than applying committed optimization tools. In addition, ADM1 is mainly applied to research purposes and may not have the same level of integration and applicability in industrial settings as commercial process simulation software such as AP. Furthermore, AP software offers several advantages over the ADM1 model. Users can easily construct and modify process models using AP's user-friendly interface and drag-and-drop functionality. These techniques enable comprehensive optimization, accommodating numerous objectives and constraints. The optimization tools in AP encompass sensitivity analysis, parameter estimation, and process design optimization. AP is widely employed in the industry, and its optimization potential makes it particularly well-suited for commercial-scale biogas generation operations. Thus, for authors primarily interested in AcoD process design and optimization within a broader context, AP proves to be a reliable choice due to its versatility and user-friendly interface [117]. However, for gaining a deep understanding of the AcoD process and making directed adjustments to the model, the modified ADM1 might be a valuable tool.

## 6. Policy Implications and Future Outlook

It has been observed that codigesting multiple substrates increases the volume of biogas output with the desired quality due to the synergistic interactive effects. Numerical simulation may help investigators in optimizing operation parameters and forecasting biogas production under different conditions. Providing such estimates and evidence may add value to the existing knowledge in academia and provide more chances for new and additional perspectives in the biogas arena to accomplish the desired biogas sector goals [141]. Thus, a review of this kind has significant policy implications for planning, implementing, and expanding

biogas plants. First, AcoD system optimization with process parameters, mathematical modeling, and simulation tools for domestic and large-scale biogas plants may help improve economic viability and account for higher biogas yield. Second, policymakers may use the results of this review to promote efficient commercial AcoD plants intensively. In addition, the dissemination of this review is likely to help local communities enhance biogas production, which in turn can increase the acceptance of biogas technology.

The developed mathematical models, however, have difficulties due to their failure to meet the initial conditions of biogas production, the complexity of the feed substrate materials, their chemical composition, and their fundamental transformation. Thus, some suggestions for further research may be emphasized as follows:

- (1) For the design and modeling of AcoD, AP, and ADM1 have taken over. However, AP is still in the simulation stage and still in its infancy. Thus, the AP software still needs a good understanding of process engineering principles and sufficient input information for precise modeling, simulation, and optimization of biogas processes.
- (2) The AcoD system requires more extensive modeling than monodigestion since it works at a high organic load with a substrate of different characteristics. Future AcoD processes simulating new models must contain new features that consider the interactions between system performances, the contents of cosubstrate, organic loading, and the inhibition level to maximize biogas yield.
- (3) The models developed to date do not consider the environmental and time-based fluctuation of substrates in biogas production simulation. Biogas models should incorporate the idea of a multistage AcoD process mechanism and include the factors that affect the products. It is realized in this study that there are still research gaps in optimizing anaerobic codigestion processes.
- (4) In addition, technoeconomic evaluation coupled with the life cycle assessment of AcoD systems may be a prerequisite for the types of feeds and related charges to recommend the premium for codigestion biorefineries and generate sufficient special information to guarantee investment for commercial scale uses and policy making. This review considered research conducted at laboratory scales as a convenience for comparison.

## 7. Conclusions

In this review, the current status, recent progress, and future outlook on biogas production with codigestion, modeling, and optimization were detailed. Control of process parameters becomes important in attaining optimal biogas yield. Since most of the previous research studies have focused on monodigestion and look at codigestion as a way forward from the recent trend to ensure sustainability, codigestion requires a great deal of further investigations on

various feedstocks with optimal mix ratios and organic loads. Modeling and optimization while integrating codigestion feedstocks as well as seasonal variations are yet to be investigated. The coupling of codigestion and model for system optimization need further exploration. Modeling of the AD process using kinetic model, artificial intelligence, and simulation software was critically reviewed with specific reference to their computational ability and limitations. Furthermore, the study examined the application of the models in anaerobic digestion, considering aspects such as flexibility, processing time, governing equations, and adaptability. Models can beneficially be employed, utilizing their predictive capability under different designs and operating conditions to enhance and optimize biogas yield. Thus, albeit to a varied degree, this review demonstrated that process modeling can significantly shorten the process development time for anaerobic substrate digestion. However, the difficulty of parameter characterization and calibration of the AP and ADM1 models increases with its rising demand and application. Thus, more research is required to provide cutting-edge methods for characterizing the chemical compositions, biodegradability, dynamic behavior of microorganisms, and intrinsic qualities of the entire AcoD system.

### Data Availability

All data, models, and codes used to support the findings of the study are available within the article.

### Conflicts of Interest

The authors declare that they have no conflicts of interest.

### Authors' Contributions

All authors made their respective contributions from the beginning of the critical review. All authors have reviewed and consented to the final published version of the manuscript.

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### Supplementary Materials

A supplementary file concerned with methodology and data filtration criteria has been provided which shall be published online along with the review article. It precisely describes how peer-reviewed journals across the globe were browsed from online databases using search keywords. An approach utilized in literature search and data filtration steps has been described with a flowchart (Figure 1). (*Supplementary Materials*)

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