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# Advances in Kinetic Modeling of Anaerobic Digestion for Chemical Recovery in Biological Wastewater Systems

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ABSTRACT

This study explores recent advances in kinetic modeling of anaerobic digestion (AD) with a focus on optimizing chemical recovery in biological wastewater treatment systems. Anaerobic digestion has emerged as a critical component of sustainable wastewater management, enabling the conversion of complex organic substrates into valuable products such as biogas, volatile fatty acids (VFAs), and nutrients. However, the nonlinear dynamics, microbial consortia interactions, and substrate variability in AD processes pose significant challenges to prediction, control, and optimization. Kinetic models serve as essential tools for understanding system behavior, improving reactor performance, and guiding the recovery of target chemicals. This review systematically examines the development and refinement of kinetic models ranging from traditional first-order and Monod-based approaches to advanced mechanistic and machine learning-driven models. Recent innovations include the integration of multi-phase reaction kinetics, dynamic substrate degradation pathways, and microbial community modeling using ADM1 (Anaerobic Digestion Model No. 1) as a foundational framework. Hybrid models combining empirical kinetics with data-driven algorithms such as artificial neural networks (ANNs), support vector machines (SVMs), and ensemble learning techniques have demonstrated superior predictive accuracy in variable wastewater environments. Special emphasis is placed on kinetic modeling for chemical recovery beyond methane, particularly for VFAs, hydrogen, and ammonia,

which are gaining attention as value-added products in circular bioeconomy systems. Model calibration and validation techniques, sensitivity analysis, and reactor configuration-specific kinetics (e.g., UASB, CSTR, and membrane bioreactors) are also critically reviewed. Challenges such as model overparameterization, data scarcity, and lack of real-time adaptability are discussed alongside emerging solutions including real-time optimization platforms and sensor integration. By consolidating theoretical advancements and application-based studies from 2000 to 2024, this work provides a roadmap for the next generation of kinetic modeling in AD systems. These models are essential for achieving efficient chemical recovery, operational resilience, and compliance with increasingly stringent environmental regulations in wastewater management.

**Keywords**: Anaerobic Digestion, Kinetic Modeling, Biological Wastewater Treatment, Volatile Fatty Acids, ADM1, Machine Learning, Biogas, Chemical Recovery, Microbial Kinetics, Circular Bioeconomy.

## 1.0. Introduction

Anaerobic digestion (AD) has long been recognized as an essential biological treatment process for wastewater management, particularly for its ability to break down organic matter in the absence of oxygen. This process is widely used in municipal and industrial wastewater treatment plants to manage sludge and organic waste, offering significant environmental benefits by reducing the volume of waste, producing biogas, and providing a sustainable means for waste-to-energy conversion (Ajayi, et al., 2020, Ikeh & Ndiwe, 2019, Orieno, et al., 2021). AD operates through a series of complex biochemical reactions carried out by diverse microbial communities, which result in the generation of biogas primarily composed of methane and carbon dioxide. This methane is a valuable renewable energy source, and its capture can be used for electricity or heat generation, contributing to sustainability goals.

In addition to biogas production, anaerobic digestion offers significant potential for chemical recovery, which has garnered increasing attention in recent years. Key chemicals such as volatile fatty acids (VFAs), ammonia, and hydrogen, which are typically produced during the digestion process, have potential applications in the production of biofuels, biodegradable plastics, and other valuable chemicals (Bristol-Alagbariya, Ayanponle & Ogedengbe, 2022, Ogunwole, et al., 2022). VFAs, for example, are precursors for the production of bioplastics and can be utilized in the manufacture of various industrial products. Ammonia recovery can assist in nutrient management, reducing the environmental impact of nitrogen discharge into water bodies, while hydrogen, a potential clean fuel, can be produced through specialized fermentation processes in anaerobic conditions. Thus, the chemical recovery aspects of AD present significant opportunities to enhance the economic feasibility and environmental performance of wastewater treatment.

Kinetic modeling plays a crucial role in understanding and optimizing the anaerobic digestion process, particularly when focusing on chemical recovery. By developing models that describe the rates of microbial growth, substrate consumption, and product formation, researchers can

gain insights into the underlying mechanisms of AD, predict system behavior, and identify optimal conditions for enhancing specific product yields. Kinetic models are essential for designing, scaling up, and operating AD systems, particularly in complex or variable wastewater environments (Ayo, et al., 2023, Elete, et al., 2023, Kokogho, et al., 2023). These models help to identify bottlenecks, optimize process parameters such as temperature, pH, and retention time, and predict the effects of different types of organic waste on the overall performance of the system.

The objective of this review is to explore recent advances in kinetic modeling related to anaerobic digestion for chemical recovery. The scope includes a discussion of the various kinetic models developed to study different aspects of AD, with a particular focus on the production of valuable chemicals such as biogas, VFAs, ammonia, and hydrogen. The review aims to highlight the state of the art in model development, identify key challenges in kinetic modeling, and suggest future research directions for optimizing anaerobic digestion processes to improve both energy recovery and chemical production. Through this review, the goal is to provide a comprehensive understanding of the role of kinetic modeling in advancing the potential of anaerobic digestion as a sustainable technology for wastewater treatment and chemical recovery.

### 2.1. Methodology

A systematic conceptual methodology was employed to evaluate and synthesize advancements in kinetic modeling of anaerobic digestion (AD) for chemical recovery in biological wastewater systems. This approach integrates theoretical insights, empirical modeling trends, and domain-specific frameworks. Initially, relevant peer-reviewed literature, doctoral dissertations, and conceptual papers were identified from academic databases and digital libraries, focusing on the intersection of anaerobic digestion, kinetic modeling, and wastewater chemical recovery. Priority was given to sources such as Adeoba (2018), Adewoyin (2022), and Afolabi & Akinsooto (2023), whose works have laid foundational and innovative contributions in modeling and material integration strategies. A multistage eligibility process was conducted to apply selection criteria based on relevance to kinetic modeling, model validation, and application in full-scale or pilot anaerobic digestion setups.

Data was extracted manually and categorized based on model type (e.g., first-order, Monod-type, ADM1), system configuration (e.g., CSTR, UASB), kinetic parameters (e.g., hydrolysis rate, decay constants), and integration capabilities with chemical recovery technologies. Particular attention was given to the role of computational tools, AI-based predictions, and hybrid frameworks such as those proposed by Agbede et al. (2023) and Elete et al. (2023). These data points were synthesized using a thematic analysis approach, identifying recurrent trends and performance metrics across model implementations. The integration of microbial kinetics, substrate transformation dynamics, and process simulation were carefully examined for alignment with both chemical recovery and environmental sustainability targets.

To ensure methodological rigor, comparative assessments were made across case studies and conceptual frameworks to evaluate model performance under variable loading conditions, microbial community shifts, and substrate heterogeneity. Model reliability was judged by its sensitivity, robustness, scalability, and validation against experimental or real-time datasets. Insights from Afeku-Amenyo et al. (2023) and Nwulu et al. (2023) were used to evaluate potential integration with carbon capture and material flow management. Ultimately, this methodology supports the formulation of a strategic outlook on kinetic model evolution, identifies critical knowledge gaps, and lays the groundwork for AI-integrated, real-time kinetic modeling in wastewater-based resource recovery.

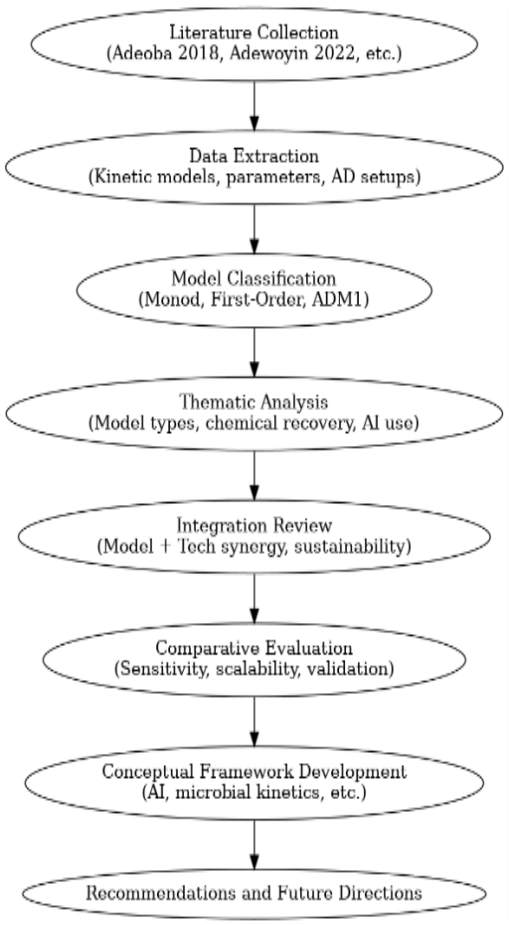


**Figure 1:** Flow chart of the study methodology

## 2.2. Fundamentals of Anaerobic Digestion Kinetics

Anaerobic digestion (AD) is a complex biochemical process in which organic matter is decomposed by microorganisms in the absence of oxygen. It is widely used in wastewater treatment and the management of organic waste because of its ability to reduce waste volume, generate biogas (primarily methane and carbon dioxide), and recover valuable chemicals. The AD process occurs in several distinct biological stages, each involving different microbial communities and specific biochemical reactions. These stages hydrolysis, acidogenesis, acetogenesis, and methanogenesis are crucial for breaking down complex organic materials and converting them into simpler compounds, such as volatile fatty acids (VFAs), ammonia, and methane. Understanding the kinetics of each stage is fundamental for optimizing the AD process, particularly when focusing on chemical recovery, as it enables the prediction of product yields and the identification of parameters that affect system performance. Figure 2 shows the techniques for improving anaerobic digestion performance presented by González, Peña & Gómez, 2022.

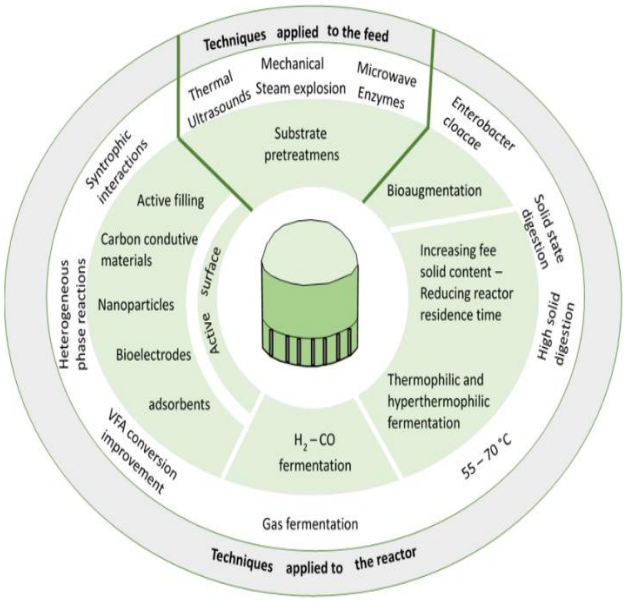


**Figure 2:** Techniques for improving anaerobic digestion performance (González, Peña & Gómez, 2022).

The first stage of anaerobic digestion, hydrolysis, involves the breakdown of complex organic polymers such as carbohydrates, proteins, and lipids into simpler monomers like sugars, amino acids, and fatty acids. This stage is typically the rate-limiting step in the overall process, as it requires the action of extracellular enzymes produced by hydrolytic bacteria. The efficiency of hydrolysis depends on several factors, including substrate concentration, enzyme availability, and the physical characteristics of the organic material (Bakare, et al., 2023, Eyeghre, et al., 2023, Lottu,et al., 2023). Acidogenesis follows hydrolysis and involves the fermentation of the simpler monomers into intermediate products such as VFAs, alcohols, and hydrogen. The acidogenic bacteria that carry out this process are facultative anaerobes, which convert the organic acids into simpler compounds such as acetic acid and hydrogen,

forming the primary substrates for the next stage of digestion. In the acetogenesis stage, acetate and hydrogen are further converted into acetic acid and additional hydrogen by acetogenic bacteria, preparing these compounds for the final step of methane production.

Methanogenesis, the last stage, is carried out by methane-producing archaea (methanogens), which convert acetic acid, hydrogen, and carbon dioxide into methane. The rate of methanogenesis is influenced by the availability of hydrogen and acetate, the most common substrates for methanogens. Methane production is typically the rate-limiting step in many AD systems, as methanogens are more sensitive to environmental conditions such as pH, temperature, and substrate concentrations than other microbial groups. As a result, maintaining the proper balance between the microbial communities in each stage is essential for optimal AD performance (Daraojimba, et al., 2021, Egbumokei, et al., 2021, Sobowale, et al., 2021).

The kinetics of anaerobic digestion have been the subject of extensive research, with many classical models developed to describe the rates of substrate consumption and product formation throughout the process. These models generally rely on mathematical equations that describe the rate of change in the concentration of substrates and products over time. The simplest and most widely used kinetic models are first-order models, which assume that the rate of substrate degradation is proportional to its concentration (Onyeke, et al., 2022, Orieno, et al., 2022, Ozobu, et al., 2022). First-order kinetics are often used in situations where the degradation rate is constant and does not vary significantly with substrate concentration, as is common in many wastewater treatment processes. Schematic representation of anaerobic digestion presented by Karuppiah & Azariah, 2019 is shown in figure 3.

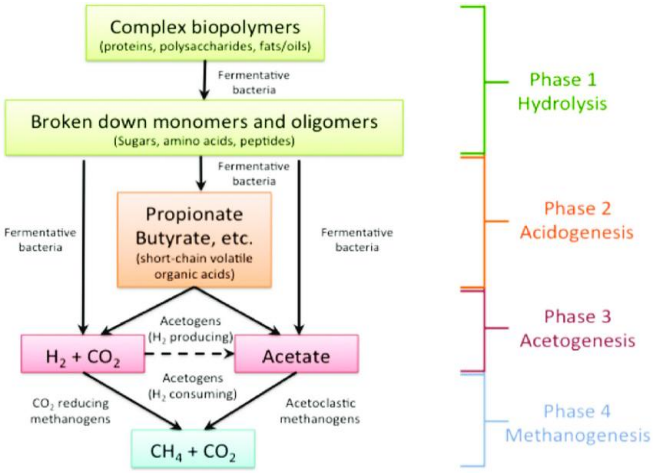


**Figure 3:** Schematic representation of anaerobic digestion (Karuppiah & Azariah, 2019).

More complex models, such as the Monod model, have been developed to account for the effects of substrate concentration on microbial growth rates. The Monod model describes microbial growth as a function of both the substrate concentration and a set of kinetic parameters, including the maximum growth rate and the half-saturation constant (Chukwuma, et al. 2022, Johnson, et al., 2022, Ogunwole, et al., 2022). The Monod equation assumes that microbial growth rates are initially high at low substrate concentrations but decrease as the substrate concentration increases, due to factors such as substrate inhibition or competition for resources. The Monod model is widely used to describe microbial kinetics in AD, particularly in systems where substrate concentration is a critical factor in determining process performance.

The Contois model is another variation of the Monod model that includes an additional term to account for biomass concentration in the system. It is particularly useful for describing systems where the growth of microorganisms is limited not only by substrate concentration but also by the availability of nutrients or other factors affecting biomass accumulation. The Contois model is used to predict microbial growth rates in systems with varying nutrient availability, where biomass concentration may not be constant over time (Akintobi, Okeke & Ajani, 2022,

Ezeanochie, Afolabi & Akinsooto, 2022). Similarly, the Grau model is often applied to describe the growth kinetics of microbial populations in AD, especially when there is a need to incorporate more detailed substrate and biomass interactions.

While classical kinetic models have provided valuable insights into the dynamics of AD, they do not fully capture the complexity of the system. Many models assume that microbial activity and substrate consumption occur at constant rates or under idealized conditions, which may not be representative of real-world AD systems. In practice, AD kinetics are influenced by a wide range of factors, including substrate composition, microbial activity, temperature, pH, and the presence of inhibitory compounds (Adeoba, 2018, Imran, et al., 2019, Orieno, et al., 2021). To better understand and predict AD performance, researchers have increasingly focused on developing more detailed and accurate models that incorporate these variables. Van, et al., 2020 presented diagram of the three-stage anaerobic digestion system shown in figure 4.

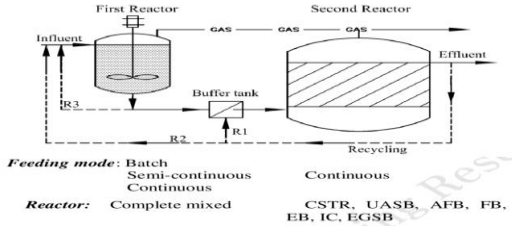


Fig. 2. The configuration of the two-stage digestion system

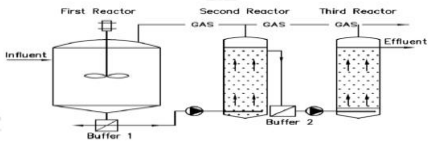


**Figure 4:** Diagram of the three-stage anaerobic digestion system (Van, et al., 2020).

One of the most significant parameters influencing AD kinetics is substrate concentration. The availability of substrate is directly related to the efficiency of the hydrolysis and acidogenesis stages, as it determines the amount of organic matter that can be converted into simpler compounds. High substrate concentrations can lead to faster reaction rates but may also result in inhibition or toxicity, particularly during acidogenesis and methanogenesis. The concentration of VFAs, for example, can inhibit methanogenic activity if they accumulate to high levels (Onukwulu, et al., 2023, Orieno, et al., 2023, Ozobu, et al., 2023). Conversely, low substrate concentrations may limit microbial growth rates and slow down the overall digestion process. Understanding how substrate concentration affects microbial kinetics is essential for optimizing AD systems and ensuring stable and efficient operation.

Microbial activity is another key factor influencing AD kinetics. The performance of the microbial communities involved in AD is highly sensitive to environmental factors such as temperature, pH, and nutrient availability. Temperature, in particular, has a strong effect on the rate of microbial metabolism, with mesophilic conditions (around 35-40°C) being most commonly used in AD systems. However, thermophilic conditions (50-60°C) can offer higher rates of digestion and enhanced pathogen reduction, although they may also require additional energy input for heating (Ojika, et al., 2021, Okolo, et al., 2021, Onukwulu, et al., 2021). pH plays a crucial role in maintaining optimal conditions for methanogens, as they are highly sensitive to acidic or alkaline environments. Typically, AD processes operate best within a narrow pH range of 6.5 to 8.0. Deviations from this range can result in reduced microbial activity, leading to slower digestion rates and lower chemical recovery.

In addition to these factors, the presence of inhibitors such as heavy metals, toxic organics, or high concentrations of ammonia can also influence AD kinetics. Ammonia toxicity, in particular, is a common challenge in industrial wastewater systems, where the accumulation of ammonia can inhibit microbial activity and reduce biogas production. Research into strategies for mitigating ammonia toxicity and enhancing the resilience of microbial communities is an important area for advancing the

efficiency of AD systems (Bristol-Alagbariya, Ayanponle & Ogedengbe, 2023, Mgbecheta, et al., 2023).

In conclusion, the kinetics of anaerobic digestion are complex and influenced by a wide range of factors that impact substrate degradation, microbial growth, and product formation. Classical kinetic models, including first-order, Monod, Contois, and Grau models, have provided foundational insights into the dynamics of AD but need to be refined to account for the multitude of variables present in real-world systems. Future research must continue to explore how substrate concentration, microbial activity, temperature, pH, and inhibitory compounds interact to shape the kinetics of anaerobic digestion. By improving our understanding of these dynamics and developing more accurate and predictive models, we can optimize AD systems for chemical recovery, enhance energy production, and improve overall wastewater treatment performance.

### 2.3. Standardized Modeling Approaches

The development of standardized modeling approaches for anaerobic digestion (AD) has advanced significantly in recent years, providing valuable insights into the complex biochemical processes involved in the treatment of wastewater and the recovery of chemicals. One of the most widely used models in this area is the Anaerobic Digestion Model No. 1 (ADM1), which serves as a foundational framework for simulating various reactor configurations and understanding the underlying mechanisms of AD. Over time, ADM1 has been refined, modified, and extended to enhance its applicability to chemical recovery processes, enabling better prediction of product yields and optimization of system performance.

ADM1 was developed by the International Water Association (IWA) to provide a standardized framework for modeling anaerobic digestion systems. The model incorporates a wide range of biochemical and microbial processes involved in the degradation of organic matter, including hydrolysis, acidogenesis, acetogenesis, and methanogenesis. It is a comprehensive, dynamic model that simulates the interactions between microorganisms, substrates, and environmental conditions within the AD process (Agho, et al., 2021, Ezeanochie, Afolabi & Akinsooto, 2021). The model is based on a series of differential equations that describe the conversion of organic matter into biogas and other by-products. It includes a detailed representation of microbial kinetics, with separate components for different microbial groups, including hydrolytic bacteria, acidogens, acetogens, and methanogens. ADM1 also accounts for the influence of environmental factors such as temperature, pH, and substrate concentration on microbial activity, providing a more realistic and predictive framework for AD systems.

However, despite its widespread use, ADM1 has certain limitations. One of the primary challenges of ADM1 is its complexity. The model incorporates a large number of parameters and requires detailed input data, making it computationally demanding and sometimes difficult to apply in practical settings. The model also assumes idealized conditions, such as a well-mixed reactor and constant feedstock composition, which may not always reflect real-world scenarios (Adikwu, et al., 2023, Elete, et al., 2023, Ndiwe, et al., 2023). Furthermore, while ADM1 is effective in simulating methane production and overall performance, it does not directly account for the recovery of specific chemicals, such as volatile fatty acids (VFAs), ammonia, and hydrogen, which are of particular interest for chemical recovery in AD systems. As a result, ADM1's application to chemical recovery requires modifications and extensions to incorporate the dynamics of these by-products.

To enhance the applicability of ADM1 for chemical recovery, several modifications and extensions have been proposed. One such modification is the inclusion of specific pathways for the production and degradation of VFAs, which are key intermediates in

AD and are of significant interest for resource recovery. VFAs, such as acetic acid, propionic acid, and butyric acid, are produced during the acidogenesis and acetogenesis stages of AD and can be recovered for use in the production of bioplastics, biofuels, and other chemicals (Egbuhuzor, et al., 2021, Isi, et al., 2021, Onukwulu, et al., 2021). By extending ADM1 to include more detailed models of VFA production and consumption, researchers can better predict the yields of these compounds and optimize the conditions for their recovery. Similarly, the extension of ADM1 to include ammonia recovery is another important modification, particularly for AD systems treating nitrogen-rich wastewater. Ammonia recovery can help reduce nitrogen discharge into water bodies and enable the reuse of ammonia as a fertilizer or feedstock for other chemical processes. Extensions to ADM1 that account for ammonia volatilization and recovery pathways allow for a more accurate representation of the nitrogen cycle within AD systems.

Hydrogen production is another area where ADM1 has been extended to support chemical recovery. While hydrogen is not typically a major product of conventional AD systems, certain configurations, such as dark fermentation, can produce hydrogen as a by-product. Extending ADM1 to include hydrogen production pathways allows for the simulation of AD systems that focus on hydrogen recovery, providing valuable insights into the potential for hydrogen as a clean fuel and chemical feedstock (Daraojimba, et al., 2022, Elete, et al., 2022, Okolo, et al., 2022). These modifications not only enhance the predictive power of ADM1 for chemical recovery but also provide a more detailed understanding of the metabolic pathways that govern the formation of these valuable by-products.

The calibration, sensitivity analysis, and validation of kinetic models, including ADM1 and its extensions, are crucial steps in ensuring their reliability and accuracy. Model calibration involves adjusting the model's parameters to match experimental data or real-world observations. This process is typically carried out by comparing the model's predictions of biogas production, VFA concentrations, and other key outputs with measured values from laboratory or pilot-scale AD systems (Adewoyin, 2021, Isi, et al., 2021, Ogunnowo, et al., 2021). Calibration ensures that the model accurately reflects the behavior of the system under different operating conditions, such as varying substrate concentrations, temperature fluctuations, and changes in pH.

Sensitivity analysis is another important aspect of model development, as it helps identify which parameters have the greatest influence on model outputs. In AD systems, several factors, such as substrate concentration, microbial growth rates, and environmental conditions, can affect the overall performance and the recovery of specific chemicals. Sensitivity analysis involves systematically varying the model's parameters and observing the impact on key outputs, such as methane production, VFA concentrations, and hydrogen yields (Bristol-Alagbariya, Ayanponle & Ogedengbe, 2022, Onukwulu, et al., 2022). By identifying the most sensitive parameters, researchers can prioritize which factors to focus on when optimizing AD systems for chemical recovery. Sensitivity analysis can also help determine the robustness of the model, highlighting areas where small changes in parameters can lead to large variations in output, and guiding further refinement of the model.

Validation is the final step in the model development process and involves comparing the model's predictions with independent experimental data that was not used during the calibration process. Validation ensures that the model can accurately predict the behavior of AD systems under a range of conditions and with different feedstocks. This step is particularly important when extending ADM1 for chemical recovery, as the model must be validated for each specific by-product of interest, such as VFAs,

ammonia, or hydrogen (Attah, et al., 2022, Elete, et al., 2022, Nwulu, et al., 2022). Validation provides confidence that the model can be used as a reliable tool for predicting chemical recovery in real-world systems and for optimizing operational parameters to maximize the recovery of these valuable by-products.

In conclusion, standardized modeling approaches, such as ADM1 and its extensions, are essential tools for advancing our understanding of anaerobic digestion and optimizing chemical recovery in biological wastewater systems. These models provide valuable insights into the complex biochemical processes involved in AD, enabling the prediction of biogas production and the recovery of valuable chemicals such as VFAs, ammonia, and hydrogen. While classical models like ADM1 are effective for simulating methane production and overall system performance, they require modifications and extensions to accurately represent the dynamics of chemical recovery. Calibration, sensitivity analysis, and validation are critical steps in ensuring the accuracy and reliability of these models. As research in this area continues, further refinements to ADM1 and other kinetic models will improve their predictive capabilities and contribute to the development of more efficient and sustainable anaerobic digestion systems for chemical recovery.

### 2.4. Advances in Hybrid and Data-Driven Modeling

Advances in the kinetic modeling of anaerobic digestion (AD) systems for chemical recovery have seen a significant shift in recent years with the integration of hybrid and data-driven modeling techniques. Traditional mechanistic models, while providing a fundamental understanding of the biochemical processes in anaerobic digestion, often face limitations in capturing the complexity and variability inherent in real-world systems. The need for more accurate and flexible models to optimize AD systems and improve chemical recovery such as biogas, volatile fatty acids (VFAs), ammonia, and hydrogen has driven the adoption of machine learning (ML) and hybrid approaches that combine the strengths of both mechanistic and data-driven techniques.

Traditional mechanistic models, such as the widely used Anaerobic Digestion Model No. 1 (ADM1), describe the biochemical and microbiological interactions involved in the degradation of organic matter in a detailed manner. These models rely on the laws of mass balance, thermodynamics, and microbial kinetics to predict the performance of AD systems. While they have been useful in understanding the fundamental processes of AD, they often suffer from certain limitations (Afolabi & Akinsooto, 2021, Ogundipe, et al., 2021). These models require a large number of parameters, many of which are difficult to estimate or measure directly. In addition, mechanistic models assume idealized conditions, such as well-mixed reactors and constant feedstock composition, which may not always reflect the dynamic and heterogeneous nature of real-world systems. Moreover, these models typically do not account for uncertainties and variations in operational conditions, such as changes in temperature, substrate composition, or microbial activity, which can significantly affect the performance of AD systems.

The limitations of traditional mechanistic models have prompted the development of hybrid and data-driven modeling approaches, which combine mechanistic knowledge with machine learning (ML) techniques. Machine learning techniques, particularly those used for pattern recognition, regression, and classification tasks, are well-suited for addressing the complexity and nonlinearity of AD systems. ML methods can help overcome the limitations of mechanistic models by learning from data and capturing patterns in system behavior that may not be easily described using traditional equations (Onukwulu, et al., 2023, Onyeke, et al., 2023, Orieno, et al., 2023). By using large datasets of

operational variables, including substrate concentrations, microbial activity, process conditions, and product yields, machine learning algorithms can model the complex relationships between these variables and provide predictions that are more accurate and robust in dynamic real-world environments.

One of the most widely used ML techniques in the modeling of AD systems is Artificial Neural Networks (ANNs). ANNs are computational models inspired by the human brain, consisting of layers of interconnected nodes that process information through weighted connections. These models excel at capturing complex nonlinear relationships between inputs and outputs, making them ideal for predicting the performance of AD systems under various conditions. In the context of AD, ANNs can be used to predict biogas production, VFA concentrations, ammonia recovery, and other key performance indicators (Agho, et al., 2022, Ezeafulukwe, Okatta & Ayanponle, 2022). By training an ANN on historical data, it becomes possible to predict system behavior under new conditions without the need for detailed mechanistic modeling. Furthermore, ANNs can be adapted to handle real-time process data, allowing for adaptive control and optimization of the AD process.

Support Vector Machines (SVMs) are another popular machine learning technique used in AD modeling. SVMs are supervised learning models that can be used for regression and classification tasks. They work by finding the hyperplane that best separates data points from different classes or predicts a continuous output. In AD systems, SVMs have been applied to predict variables such as methane production and substrate degradation rates, as well as to classify different types of organic waste based on their biodegradability. SVMs offer several advantages, including their ability to handle high-dimensional datasets and provide robust predictions even with small amounts of data (Daraojimba, et al., 2022, Kanu, et al., 2022, Okolo, et al., 2022). They also have the capacity to model complex, nonlinear relationships between inputs and outputs, making them useful for predicting system performance under varying operational conditions.

Random forests and ensemble methods are other data-driven techniques that have been increasingly applied in AD modeling. Random forests are a type of ensemble learning method that combines multiple decision trees to improve prediction accuracy. Each decision tree in a random forest is trained on a random subset of the data, and the final prediction is made by averaging the outputs of all the trees. Random forests are known for their ability to handle large datasets with many features, making them well-suited for modeling AD systems with multiple input variables, such as substrate concentration, pH, temperature, and microbial activity (Ojika, et al., 2021, Onaghinor, et al., 2021, Sobowale, et al., 2021). Ensemble methods, including boosting and bagging techniques, have also been used to combine multiple models to improve predictive accuracy and reduce overfitting.

One of the most promising developments in AD modeling is the integration of hybrid frameworks that combine mechanistic models with machine learning techniques. These hybrid models aim to leverage the strengths of both approaches, combining the mechanistic understanding of AD processes with the predictive power of data-driven methods. The mechanistic component of the model provides a structured framework for describing the underlying biochemical processes, while the machine learning component captures the complex, nonlinear relationships between input variables and system outputs (Akintobi, Okeke & Ajani, 2023, Eyeghre, et al., 2023, Ogunwole, et al., 2023). Hybrid models can help improve the accuracy of predictions, especially in cases where traditional mechanistic models fail to capture the full range of system dynamics. For example, a hybrid model might use a mechanistic model to simulate the degradation of organic matter

in the AD system, while using machine learning algorithms to predict the production of VFAs or ammonia recovery based on process data.

These hybrid models also offer the advantage of adaptability. As new data becomes available from operational systems, the machine learning component can be updated to improve the model's predictions. This adaptability allows the model to account for changing conditions, such as variations in feedstock composition or fluctuations in operational parameters like temperature and pH. Moreover, hybrid models can be used to optimize AD systems in real-time, providing operators with actionable insights that can be used to adjust process conditions and maximize chemical recovery (Bristol-Alagbariya, Ayanponle & Ogedengbe, 2023, Nwakile,et al., 2023). For instance, machine learning algorithms can be used to optimize substrate feed rates, microbial inoculation strategies, or temperature control, ensuring that the AD system operates at its highest efficiency.

Case studies have demonstrated the effectiveness of hybrid and data-driven models in improving the prediction accuracy and control of AD systems. For example, one study applied an ANN-based model to predict the methane production rate in a large-scale anaerobic digester fed with food waste. The model successfully predicted the methane yield based on parameters such as substrate concentration, pH, temperature, and hydraulic retention time (HRT). By using real-time data, the model was able to adapt to changes in feedstock quality and operational conditions, improving system stability and efficiency (Ajayi, et al., 2021, Odio, et al., 2021, Onukwulu, et al., 2021). Another case study used a random forest-based model to predict VFA production in a continuous AD system. The model outperformed traditional mechanistic models, providing more accurate predictions and allowing for better control of VFA recovery. These examples demonstrate the potential of hybrid and data-driven modeling to enhance the performance of AD systems, particularly for chemical recovery, by improving predictions, optimizing operational conditions, and enabling real-time control.

In conclusion, the integration of machine learning techniques with traditional mechanistic models represents a major advancement in the kinetic modeling of anaerobic digestion for chemical recovery. Machine learning methods, such as ANNs, SVMs, and random forests, offer the ability to model complex, nonlinear relationships in AD systems, improving prediction accuracy and providing a powerful tool for optimization and control (Edwards & Smallwood, 2023, Elete, et al., 2023, Nwulu, et al., 2023). Hybrid modeling frameworks that combine mechanistic models with machine learning techniques hold great promise for enhancing the performance of AD systems, particularly in the context of chemical recovery. By incorporating real-time data and enabling adaptive control, these models can improve biogas production, VFA recovery, ammonia recovery, and hydrogen production. The continued development of hybrid and data-driven models will play a crucial role in optimizing anaerobic digestion systems, improving resource recovery, and advancing the sustainability of wastewater treatment processes.

### 2.5. Modeling for Targeted Chemical Recovery

Modeling for targeted chemical recovery in anaerobic digestion (AD) systems is an essential component in optimizing the efficiency of wastewater treatment while simultaneously recovering valuable chemicals such as volatile fatty acids (VFAs), hydrogen, and ammonia. These chemicals have significant applications in various industries, including the production of biofuels, biodegradable plastics, fertilizers, and other high-value products. Traditional anaerobic digestion models, primarily designed to simulate biogas production, do not always provide the resolution necessary for targeted chemical recovery. Therefore, specialized modeling approaches are

required to optimize the conditions for specific chemical production within anaerobic digestion systems, enabling the efficient extraction of these valuable products.

One of the key areas of focus in modeling for targeted chemical recovery is the production and optimization of volatile fatty acids (VFAs), which are key intermediates in the anaerobic digestion process. VFAs, including acetic acid, propionic acid, butyric acid, and others, are produced during the acidogenesis stage of AD, and their concentrations can significantly affect the overall process (Afeku-Amenyo, et al., 2023, Fiemotongha, et al., 2023, Sobowale, et al., 2023). Modeling VFAs production involves understanding the microbial kinetics of acidogenic bacteria, which convert organic matter into VFAs. Several kinetic models have been developed to describe the production of VFAs in AD, often building upon basic Monod kinetics or more complex approaches that account for substrate inhibition, pH effects, and microbial competition.

To optimize VFA production, it is essential to model not only the substrate degradation but also the metabolic pathways and the microbial populations involved. The concentration of VFAs is influenced by several factors, including the feedstock composition, the residence time in the reactor, temperature, and pH. Through targeted modeling, these factors can be adjusted to favor the production of specific VFAs. For example, acetic acid is a key substrate for methanogenesis, so its production needs to be carefully managed to prevent inhibition of methane-producing bacteria (Ayo-Farai, et al., 2023, Ezeanochie, Afolabi & Akinsooto, 2023). Conversely, optimizing the production of butyric or propionic acid may be desirable for applications such as bioplastics or biodegradable surfactants. By simulating different operational conditions, such as adjusting the pH or controlling the retention time, modelers can optimize VFA yields and ensure that the desired VFA profiles are achieved.

Similarly, modeling the production of hydrogen in anaerobic digestion systems has gained significant attention due to its potential as a clean and renewable fuel. Hydrogen is produced through dark fermentation in AD, a process where certain types of bacteria ferment organic substrates in the absence of oxygen. The production of hydrogen is often hindered by inhibitory factors such as high concentrations of fatty acids, which can accumulate during acidogenesis. Modeling hydrogen production kinetics requires a detailed understanding of the fermentation process, including the hydrogenase activity of hydrogen-producing bacteria and the competition between different microbial populations for substrates (Bristol-Alagbariya, Ayanponle & Ogedengbe, 2022, Ogunnowo, et al., 2022). Kinetic models for hydrogen production must account for factors such as substrate concentration, microbial growth rates, and the influence of environmental conditions like pH and temperature on microbial activity. By optimizing these factors through modeling, it is possible to enhance hydrogen yields while minimizing unwanted side reactions, such as the production of VFAs or methane. These models also help identify the optimal conditions for hydrogen production, such as the best type of organic feedstock, the appropriate reactor configuration, and the ideal operating conditions.

Ammonia production is another area of interest in anaerobic digestion, particularly when the treatment of nitrogen-rich wastewater is involved. Ammonia can be recovered and used as a fertilizer, providing an economic benefit while reducing the environmental impact of nitrogen discharge into water bodies. The kinetics of ammonia production in AD are influenced by both the microbial processes and the physicochemical conditions within the reactor (Adeoba & Yessoufou, 2018, Oyedokun, 2019, Uzozie, et al., 2023). In the first stages of digestion, ammonia is released from proteins and amino acids through deamination. However, excessive ammonia

concentrations can inhibit the activity of methanogens and slow down the digestion process. In addition to its role in the microbial breakdown of nitrogen-containing compounds, ammonia recovery is also affected by temperature, pH, and the type of organic waste being processed. Modeling the production and recovery of ammonia in AD requires understanding the complex interactions between microbial populations and environmental conditions. By simulating these interactions, models can predict ammonia production rates and help optimize the operational conditions, such as pH adjustments or temperature control, to enhance ammonia recovery without adversely affecting the overall digestion process.

Reactor-specific modeling plays a crucial role in optimizing targeted chemical recovery in AD systems. Different reactor configurations, such as Upflow Anaerobic Sludge Bed (UASB) reactors, Continuous Stirred-Tank Reactors (CSTR), and Anaerobic Membrane Bioreactors (AnMBR), have distinct advantages for different types of chemical recovery, and each reactor type responds differently to operational conditions. For example, UASB reactors are commonly used for high-strength wastewater treatment and offer a high hydraulic retention time, which is advantageous for the production of methane and other gases (Onukwulu, et al., 2023, Onyeke, et al., 2023, Ozobu, et al., 2023). However, the high concentration of sludge and solids in UASB reactors may limit the recovery of certain chemicals, such as VFAs, due to the high microbial density and low substrate availability in the liquid phase. CSTR reactors, on the other hand, provide more uniform mixing, which can lead to better control over microbial populations and higher rates of chemical recovery. However, they may require more complex operational control and monitoring due to their larger size and more dynamic conditions.

Anaerobic Membrane Bioreactors (AnMBRs) combine anaerobic digestion with membrane filtration, providing the advantage of concentrating biomass and effluent, which can enhance chemical recovery efficiency. However, the fouling of membranes and the need for regular cleaning can be operational challenges. Modeling these different reactor types for chemical selectivity requires a detailed understanding of the mass transfer, microbial kinetics, and hydrodynamics within each reactor (Ojika, et al., 2023, Okolo, et al., 2023, Okuh, et al., 2023). For instance, in AnMBRs, the modeling would need to account for both the filtration process and the anaerobic degradation process, optimizing the membrane flux while ensuring maximum recovery of VFAs, hydrogen, and ammonia. Reactor-specific models help identify which configuration is most suitable for a given substrate or chemical recovery target, ensuring that the system operates at peak efficiency.

The impact of operational conditions on chemical yields is another critical area of research. Factors such as temperature, pH, substrate concentration, retention time, and mixing rates all influence the efficiency of anaerobic digestion and chemical recovery. For example, temperature directly affects the metabolic rates of microbes and the solubility of gases, such as hydrogen. Mesophilic conditions (around 35-40°C) are commonly used in AD systems, but thermophilic conditions (50-60°C) can increase the rate of digestion and enhance pathogen removal (Adewoyin, 2022, Elete, et al., 2022, Nwulu, et al., 2022). However, thermophilic conditions can also cause the accumulation of inhibitory compounds, such as ammonia and VFAs, which can hinder chemical recovery. By modeling the effects of temperature and other operational factors on chemical yields, researchers can identify the optimal conditions for maximizing the recovery of target chemicals while minimizing the formation of inhibitory by-products.

Additionally, pH plays a crucial role in the microbial metabolism and product formation in AD systems.

Methanogens, for example, are sensitive to acidic conditions, and their activity can be inhibited when the pH drops below a certain threshold. On the other hand, the acidogenesis and acetogenesis stages may benefit from slightly acidic conditions, which can enhance VFA production. By modeling the effects of pH on the microbial populations and their metabolic pathways, it is possible to determine the optimal pH range for chemical recovery in specific AD systems (Afolabi & Akinsooto, 2023, Hanson, et al., 2023, Ogunwole, et al., 2023). Similarly, substrate concentration, microbial activity, and mixing intensity all interact to influence the yield of chemicals in the system. Simulation models that integrate these variables provide a powerful tool for optimizing the operational parameters in AD systems for targeted chemical recovery.

In conclusion, modeling for targeted chemical recovery in anaerobic digestion is an essential tool for optimizing the process and improving the yields of valuable chemicals such as volatile fatty acids, hydrogen, and ammonia. By understanding and simulating the microbial kinetics, reactor configurations, and operational conditions, researchers can develop more efficient and sustainable AD systems. Advances in modeling techniques, including the development of reactor-specific models and the optimization of operational conditions, will help improve the chemical recovery potential of anaerobic digestion and contribute to the broader goals of resource recovery and waste management. These models offer valuable insights into the dynamics of AD, enabling operators to tailor the system to maximize chemical production while ensuring the stability and efficiency of the digestion process.

### 2.6. Real-Time Modeling, Monitoring, and Control

I Real-time modeling, monitoring, and control in anaerobic digestion (AD) systems have gained significant importance in recent years, particularly for chemical recovery in biological wastewater treatment. These advancements aim to enhance the efficiency of AD processes and optimize the production of valuable chemicals, such as biogas, volatile fatty acids (VFAs), hydrogen, and ammonia, by responding dynamically to changing system conditions. The integration of real-time data acquisition systems, model-predictive control (MPC), and digital twins offers a powerful approach for optimizing AD performance, making it possible to operate systems at peak efficiency and achieve better chemical recovery outcomes. However, the real-time implementation of these technologies also presents several challenges, including the need for accurate modeling, robust sensor integration, and continuous adaptation to changing operational conditions.

The integration of sensors and real-time data acquisition is a critical aspect of optimizing AD processes. Sensors play a crucial role in monitoring key parameters that directly influence microbial activity and chemical production in anaerobic digestion, such as temperature, pH, dissolved oxygen (DO), substrate concentration, and biogas production. These sensors provide real-time data that can be used to assess the performance of the system, detect anomalies, and make adjustments to optimize conditions for microbial growth and chemical recovery (Daraojimba, et al., 2023, Gidiagba, et al., 2023, Onukwulu, et al., 2023). For example, monitoring the pH and temperature in real-time allows for quick intervention to maintain the optimal environment for methanogens and other microbial communities involved in the digestion process. Sensors that measure substrate concentrations or gas production rates enable operators to track the degradation of organic matter and the production of biogas and volatile fatty acids, providing valuable information for fine-tuning the process.

Real-time data acquisition is not only valuable for process optimization but also for predictive modeling and adaptive control. The continuous flow of data

from sensors can be used to update dynamic models of the AD system in real time, providing a more accurate and up-to-date representation of system behavior. For example, the concentration of volatile fatty acids, ammonia, or hydrogen can fluctuate depending on various operational conditions, such as feedstock variability, retention time, and temperature (Banso, et al., 2023, Ezeanochie, Afolabi & Akinsooto, 2023). By using real-time data to update kinetic models, operators can predict how these fluctuations will impact the overall system performance, allowing for more precise adjustments to operational parameters, such as substrate feed rates or reactor conditions. This real-time feedback loop enables operators to optimize the recovery of valuable chemicals, ensuring that the AD process operates at its highest efficiency and that by-products such as VFAs, hydrogen, and ammonia are recovered at optimal levels.

Model-predictive control (MPC) is another key technology that has emerged in the field of AD modeling, providing a powerful tool for real-time optimization and control. MPC involves using dynamic models of the system to predict future behavior and optimize control inputs, such as substrate feeding, temperature regulation, or pH adjustments. MPC is based on the concept of solving an optimization problem at each time step, where the model predicts the future evolution of the system based on current and past data, and control inputs are adjusted to minimize an objective function, such as maximizing chemical recovery or biogas production (Bristol-Alagbariya, Ayanponle & Ogedengbe, 2023, Ogunnowo, et al., 2023). In the context of AD, MPC can be used to optimize operational parameters in real time, improving system stability and chemical recovery rates while minimizing the formation of inhibitory by-products, such as ammonia or volatile fatty acids. By continuously updating the model with real-time data, MPC ensures that the system responds to changes in feedstock composition, microbial activity, and environmental conditions, thereby enhancing the overall performance of the AD process.

One of the most exciting advancements in real-time modeling and control for AD systems is the use of digital twins. A digital twin is a virtual representation of a physical system that is continuously updated with real-time data from sensors and other sources. In the case of AD systems, a digital twin can simulate the behavior of the biological processes and predict how changes in operational conditions will affect chemical recovery and system performance. Digital twins can be integrated with real-time data acquisition systems and model-predictive control frameworks to provide a comprehensive, real-time simulation of the AD process (Agho, et al., 2023, Ezeamii, et al., 2023, Ogu, et al., 2023). These digital models allow operators to test different control strategies and optimize system performance without disrupting the actual system, making it possible to simulate "what-if" scenarios and predict the impact of process changes before they are implemented in the physical system. For example, digital twins can simulate the effects of temperature fluctuations or substrate composition on methane production or VFA recovery, helping operators identify optimal operating conditions. Furthermore, the integration of machine learning with digital twins can enhance predictive capabilities, enabling the system to adapt and improve over time as more data is collected and analyzed.

Despite the many advantages of real-time modeling, monitoring, and control, several challenges remain in their implementation and adaptive modeling. One of the primary challenges is the accuracy and reliability of sensor data. In anaerobic digestion systems, which are highly dynamic and often subject to fluctuations in feedstock quality and microbial activity, obtaining accurate and consistent measurements is critical for effective real-time monitoring and control. Sensors must be carefully calibrated to ensure that they provide reliable data over time, and they must be able

to operate in harsh environments, such as high temperatures, low pH, and the presence of contaminants (Akintobi, Okeke & Ajani, 2022, Kanu, et al., 2022, Onukwulu, et al., 2022). Moreover, the sensors must be capable of measuring key parameters at the appropriate temporal resolution, ensuring that changes in the system can be detected and addressed quickly.

Another challenge in the implementation of real-time monitoring and control is the complexity of integrating the sensor data with kinetic models and control algorithms. Real-time data acquisition systems generate large amounts of data, which must be processed and analyzed in real time to provide actionable insights. The integration of these data with dynamic models requires the development of advanced data processing and modeling techniques that can handle large datasets and provide predictions that are both accurate and timely (Ajayi, et al., 2023, Isong, et al., 2023, Nwulu, et al., 2023). In addition, there must be a robust feedback loop between the model, control system, and physical AD system to ensure that operational adjustments are made based on real-time predictions. This integration requires sophisticated computational tools and algorithms that can process the data efficiently and support decision-making in real-time.

Adaptive modeling is another key challenge in real-time implementation. AD systems are subject to many uncertainties, including variability in feedstock composition, changes in microbial populations, and fluctuations in environmental conditions. These uncertainties can make it difficult to accurately predict system behavior using static models. To address this, adaptive modeling approaches are needed that can update model parameters dynamically based on real-time data and system feedback (Edwards, Mallhi & Zhang, 2018, Tula, et al., 2004, Vindrola-Padros & Johnson, 2022). These models must be able to account for the nonlinearity and complexity of the biological processes involved in AD, as well as the interactions between different microbial communities and environmental factors. Developing adaptive models that can continuously learn from new data and adjust their predictions accordingly is a critical challenge in the real-time optimization of AD systems.

Finally, real-time implementation and adaptive modeling must be accompanied by the development of user-friendly interfaces and decision-support tools that allow operators to interact with the system and make informed decisions. The ability to visualize real-time data, model predictions, and control actions in an intuitive manner is essential for operators to effectively manage AD systems. These tools must be designed to provide clear insights into system performance and enable quick interventions when necessary (Ojika, et al., 2023, Okolo, et al., 2023, Olurin,et al., 2023).

In conclusion, real-time modeling, monitoring, and control are essential for optimizing anaerobic digestion systems for chemical recovery. By integrating sensors, model-predictive control, and digital twins, operators can monitor system performance in real time, optimize operational conditions, and enhance the recovery of valuable chemicals such as biogas, VFAs, hydrogen, and ammonia. These technologies offer significant potential for improving the efficiency and sustainability of AD systems. However, challenges related to sensor reliability, data integration, adaptive modeling, and user interfaces must be addressed to ensure the successful implementation of real-time optimization and control in anaerobic digestion processes. As these challenges are overcome, real-time modeling and control will play a key role in the development of more efficient, sustainable, and resource-efficient wastewater treatment systems.

### 2.7. Challenges and Limitations

The application of kinetic modeling in anaerobic digestion (AD) for chemical recovery in biological

wastewater systems has advanced significantly in recent years. While these models have enhanced our understanding of the complex biochemical processes involved in AD, they also come with challenges and limitations that need to be addressed to ensure their successful implementation and optimization in real-world systems. As AD becomes increasingly vital for wastewater treatment and resource recovery, particularly in the production of chemicals such as volatile fatty acids (VFAs), hydrogen, and ammonia, the need for accurate, reliable, and scalable models grows. Despite the potential benefits, several hurdles remain, including issues related to data quality and availability, model overfitting and parameter identifiability, and difficulties in scaling up models to diverse and complex wastewater streams.

Data quality and availability are fundamental challenges in the development and application of kinetic models for anaerobic digestion. Accurate modeling requires high-quality, comprehensive datasets that represent the complex dynamics of the AD process, including microbial growth rates, substrate degradation, product formation, and the influence of operational parameters such as temperature, pH, and hydraulic retention time (HRT) (Bristol-Alagbariya, Ayanponle & Ogedengbe, 2022, Onukwulu, et al., 2022). However, in practice, obtaining reliable and consistent data from real-world AD systems is often difficult. The quality of data may be compromised by sensor limitations, measurement errors, or inconsistencies in data collection protocols. In addition, the variability of feedstock, the dynamic nature of microbial populations, and the presence of inhibitors or contaminants further complicate the collection of accurate data.

The scarcity of high-quality data is particularly problematic when it comes to chemical recovery. To optimize the production of valuable by-products such as VFAs, ammonia, and hydrogen, it is essential to understand the kinetic parameters that govern their formation and consumption throughout the AD process. However, many of these parameters are difficult to measure directly, requiring the use of proxies or indirect methods. For example, the concentration of VFAs or hydrogen may fluctuate over time due to changes in microbial activity, temperature, or substrate availability, making it challenging to obtain stable data for model calibration (Adeoba, etal., 2018, Omisola, et al., 2020, Uzozie, et al., 2023). Inadequate or unreliable data may lead to inaccurate predictions, limiting the model's ability to optimize AD performance and chemical recovery.

Another significant challenge in kinetic modeling of AD is model overfitting and parameter identifiability. Overfitting occurs when a model becomes too complex or is excessively tuned to match a specific dataset, leading to predictions that are accurate for the given data but fail to generalize to new or unseen conditions. This issue arises because kinetic models often contain numerous parameters, many of which are difficult to estimate or quantify. As a result, the model may become overly sensitive to small variations in the data, leading to unrealistic or non-representative predictions. Overfitting can lead to misleading results, particularly when trying to extrapolate model predictions to different operational conditions or wastewater types (Daraojimba, et al., 2023, Ezeh,et al., 2023, Olurin,et al., 2023).

Parameter identifiability refers to the difficulty of determining unique values for the model parameters based on available data. In many cases, AD models include a large number of parameters, such as microbial growth rates, substrate consumption rates, and yield coefficients, which are not easily measured or directly observed. When multiple parameters influence a given system behavior, it can be challenging to identify the exact values of those parameters. This lack of identifiability can lead to

model uncertainty, making it difficult to optimize AD systems for specific chemical recovery goals (Adeoba, Tesfamichael & Yessoufou, 2019, Ubamadu, et al., 2023). In addition, uncertainty in parameter estimation can propagate through the model, leading to unreliable predictions and suboptimal control decisions. Researchers must therefore use advanced techniques such as sensitivity analysis, Bayesian methods, or optimization algorithms to improve parameter identifiability and reduce model uncertainty.

The scalability of kinetic models and their applicability to diverse wastewater streams is another major challenge in the modeling of anaerobic digestion for chemical recovery. While many kinetic models have been successfully applied to small-scale or laboratory-based AD systems, translating these models to larger, more complex systems presents significant difficulties. Scaling up models involves accounting for the increased complexity of real-world systems, which may include variations in feedstock composition, microbial populations, reactor configurations, and operational conditions (Onukwulu, et al., 2023, Onyeke, et al., 2023, Oyeyipo, et al., 2023). As the size and complexity of the AD system increase, so too does the number of variables that must be considered, leading to greater uncertainties in model predictions.

Wastewater streams are highly variable in their composition, which adds another layer of complexity to scaling up kinetic models. Different wastewater streams, such as municipal sewage, agricultural runoff, or industrial effluents, contain distinct concentrations of organic matter, nutrients, and contaminants. These differences can significantly affect the microbial dynamics within the reactor and the production of specific chemicals. For instance, wastewater from food processing plants may be rich in carbohydrates, while industrial effluents may contain high levels of heavy metals or toxic compounds (Agbede, et al., 2023, Iwe, et al., 2023, Obianyo & Eremeeva, 2023). As a result, a model that is calibrated for one type of wastewater may not be applicable to another without significant adjustments or recalibrations. The heterogeneity of wastewater streams also makes it challenging to develop generalized models that can accurately predict chemical recovery across a wide range of systems and feedstocks.

The issue of scaling up is further compounded by the fact that many AD models, including those for chemical recovery, are based on idealized conditions that may not reflect the complexities of real-world operations. In laboratory-scale systems, conditions such as temperature, pH, and substrate concentration can be carefully controlled, allowing for a more predictable and stable system. However, in larger, field-scale systems, these conditions can fluctuate significantly, making it more difficult to maintain the optimal conditions for chemical production (Bristol-Alagbariya, Ayanponle & Ogedengbe, 2023, Nwulu, et al., 2023). As a result, scaling up kinetic models to real-world applications requires the inclusion of additional factors, such as reactor geometry, hydrodynamics, and mass transfer limitations, which may not have been considered in smaller-scale models.

Another challenge in scaling up is the integration of the kinetic models with real-time monitoring and control systems. For large-scale AD systems, continuous monitoring of key parameters such as temperature, pH, and gas production is essential for maintaining optimal process conditions. However, real-time data acquisition in large systems often generates vast amounts of data that must be processed and analyzed quickly to inform control decisions. The integration of these real-time data streams with kinetic models requires advanced computational tools and algorithms that can handle large datasets and provide actionable insights in real-time (Ajiga, Ayanponle & Okatta, 2022, Noah, 2022, Ogundipe,

Sangoleye & Udokanma, 2022). This can be especially challenging when dealing with complex or heterogeneous feedstocks that introduce variability into the system.

Finally, the adaptation of kinetic models to diverse wastewater streams and large-scale systems requires extensive experimental validation. To ensure that models accurately predict system performance and chemical recovery, they must be validated against real-world data from a variety of operational conditions and feedstock types. This validation process can be time-consuming and resource-intensive, as it requires collecting large amounts of experimental data and performing rigorous model comparisons (Akintobi, Okeke & Ajani, 2023, Izuka, et al., 2023, Onukwulu, et al., 2023). Without proper validation, the reliability and accuracy of the model predictions may be compromised, leading to suboptimal decision-making and reduced chemical recovery efficiency.

In conclusion, while kinetic modeling has the potential to significantly improve the efficiency of anaerobic digestion systems for chemical recovery, several challenges and limitations remain. Issues related to data quality and availability, model overfitting, parameter identifiability, and scalability must be addressed to ensure that these models can be effectively applied to real-world systems. Overcoming these challenges requires advancements in sensor technology, model calibration techniques, and computational tools to enhance model accuracy and reliability. Additionally, further research is needed to develop more robust and generalized models that can handle the variability and complexity of different wastewater streams and operational conditions. By addressing these challenges, the field of kinetic modeling for chemical recovery in anaerobic digestion can continue to evolve and provide valuable insights into optimizing waste-to-energy systems and resource recovery processes.

### 2.8. Future Directions

The future directions of kinetic modeling in anaerobic digestion (AD) systems, particularly for chemical recovery in biological wastewater systems, promise significant advancements that could lead to more efficient, sustainable, and scalable processes. These developments will not only improve the understanding of complex microbial dynamics but also optimize the production of valuable chemicals such as volatile fatty acids (VFAs), hydrogen, methane, and ammonia. As the need for sustainable waste management and resource recovery continues to grow, future advances in kinetic modeling will play a crucial role in revolutionizing the way we approach wastewater treatment and resource recovery.

One of the most promising future directions for kinetic modeling in AD systems is the development of fully autonomous, AI-driven systems. The integration of artificial intelligence (AI) and machine learning (ML) with AD kinetic models has the potential to transform the way these systems are operated and optimized. AI-driven systems can continuously analyze large volumes of real-time data collected from sensors embedded within the AD system, allowing for adaptive control and optimization of operational conditions without human intervention (Onaghinor, et al., 2021, Orieno, et al., 2022, Sobowale, et al., 2022). For example, AI algorithms can predict and adjust parameters such as temperature, pH, substrate feed rates, and retention times to optimize the yield of desired products, such as VFAs or methane. These systems would not only improve the overall efficiency of AD systems but also reduce operational costs by minimizing energy consumption, labor requirements, and waste generation. Furthermore, AI-driven models can learn from historical data and past system performance, continuously improving their predictions and optimization strategies over time.

The coupling of kinetic models with microbial genomics and community dynamics is another promising avenue for advancing AD modeling. Traditional kinetic models primarily focus on the rates of substrate consumption and product formation, often treating microbial populations as homogeneous groups with fixed metabolic pathways. However, in reality, the microbial community in AD systems is highly diverse and dynamic, with different species interacting in complex ways. Advances in microbial genomics and metagenomics have enabled the identification and characterization of the microbial communities involved in AD, providing new insights into their metabolic capabilities and interactions (Onyeke, et al., 2022, Orieno, et al., 2021, Ubamadu, et al., 2023). By integrating kinetic models with genomic data, researchers can develop more accurate representations of microbial community dynamics, allowing for better predictions of system behavior and improved optimization of chemical recovery. For example, understanding the specific microbial species responsible for the production of VFAs, hydrogen, or methane can help target operational conditions that favor the growth of beneficial microbes, leading to enhanced recovery of desired products. Additionally, by studying microbial interactions, researchers can identify potential inhibitors or competitive interactions that may reduce the efficiency of chemical recovery and take steps to mitigate these issues.

The future of AD kinetic modeling will also involve the development of standardized, open-access kinetic platforms that can be used by researchers, engineers, and operators across the world. Standardization is essential to ensure that models are widely applicable, reproducible, and easy to integrate into various AD systems, regardless of location or scale. An open-access platform would allow stakeholders from academia, industry, and government to collaborate and contribute to the development of more accurate and generalized models, accelerating progress in the field (Ojika, et al., 2023, Ojo, et al., 2023, Okolo, et al., 2023). These platforms would provide a user-friendly interface for the development, calibration, and validation of kinetic models, enabling researchers to build upon existing models and share data and insights. In particular, such platforms would allow for the integration of diverse datasets from different types of wastewater, operational conditions, and reactor configurations, leading to more robust and generalized models that can be applied to a wider range of systems. Moreover, by making kinetic models and simulation tools openly available, the scientific community can accelerate the process of optimization and innovation, facilitating the adoption of advanced AD technologies globally.

Furthermore, as the field of AD modeling continues to evolve, there will likely be a greater focus on the development of multi-scale models that can simulate the behavior of AD systems at different levels of complexity. These models would integrate molecular, microbial, reactor, and system-level dynamics to provide a comprehensive understanding of the AD process. For instance, at the molecular level, models could simulate the biochemical reactions that occur during hydrolysis, acidogenesis, acetogenesis, and methanogenesis, providing detailed insights into the metabolic pathways and enzymatic reactions involved. At the microbial level, models could simulate the interactions between different microbial species and their impact on substrate degradation and product formation (Egbuhuzor, et al., 2023, Fiemotongha, et al., 2023, Nwulu, et al., 2023). At the reactor level, models could incorporate factors such as mixing, temperature gradients, and mass transfer limitations, while system-level models could consider the influence of external variables such as feedstock variability, nutrient availability, and environmental conditions. By integrating these different levels of modeling, researchers would be able to develop more accurate and predictive models that can be used to

optimize chemical recovery and process performance across a wide range of AD systems.

As the demand for chemical recovery and resource recovery grows, kinetic modeling in AD will also need to incorporate the recovery of a broader range of chemicals, including biofuels, bioplastics, and other high-value products. For example, the production of bioplastics from VFAs produced during AD has gained increasing attention due to the growing need for sustainable alternatives to petroleum-based plastics. Future models will need to focus on optimizing the conditions for the production of such chemicals while maintaining the overall efficiency of the AD process (Agho, et al., 2023, Ezeamii, et al., 2023, Nwankwo & Etukudoh, 2023). This may require the integration of additional models or simulations to account for the downstream processing of the recovered chemicals, such as purification, separation, and conversion processes. Additionally, future models will need to incorporate the economic and environmental sustainability aspects of chemical recovery, including lifecycle assessments (LCA), cost-benefit analyses, and emissions reductions, to ensure that the recovery of chemicals from AD is economically viable and environmentally sound.

One of the key challenges in the future development of AD models is the need to incorporate greater uncertainty into the models. Real-world AD systems are subject to a wide range of uncertainties, including variations in feedstock composition, microbial populations, operational parameters, and environmental conditions. These uncertainties can lead to unpredictable system behavior and suboptimal performance. Future modeling approaches will need to address these uncertainties by incorporating stochastic elements or probabilistic methods into the models (Ajayi, et al., 2020, Ofori-Asenso, et al., 2020). By accounting for variability and uncertainty, models will be better equipped to predict system behavior under a wide range of operating conditions and provide more reliable optimization strategies.

Finally, one of the most exciting future directions for kinetic modeling in AD is the integration of AD systems with other waste-to-resource technologies, such as microbial fuel cells (MFCs) or electrodialysis systems. These integrated systems have the potential to recover additional chemicals or generate energy in ways that are not possible with standalone AD systems. For instance, microbial fuel cells can convert the electrons produced by microbial metabolism into electricity, creating a dual-function system that simultaneously treats wastewater and generates power (Bristol-Alagbariya, Ayanponle & Ogedengbe, 2022, Nwulu, et al., 2022). Integrating such technologies into AD systems presents new challenges for kinetic modeling, requiring the development of models that can simulate the interactions between multiple processes and predict their combined performance. This interdisciplinary approach will be crucial for the development of future AD systems that are capable of maximizing both energy recovery and chemical production.

In conclusion, the future of kinetic modeling in anaerobic digestion for chemical recovery in biological wastewater systems holds great promise for advancing the efficiency and sustainability of waste-to-resource technologies. By leveraging advances in artificial intelligence, microbial genomics, and open-access platforms, future models will be better equipped to predict system behavior, optimize chemical recovery, and scale up AD systems for diverse wastewater streams (Ayo-Farai, et al., 2023, Ezeanochie, Afolabi & Akinsooto, 2023). As the field continues to evolve, multi-scale models, greater consideration of uncertainty, and the integration of AD with other waste-to-resource technologies will be key to unlocking the full potential of anaerobic digestion for chemical recovery. Through these advancements, kinetic modeling will play a pivotal role in achieving more sustainable and efficient

wastewater treatment systems, contributing to the global effort to reduce waste, recover resources, and mitigate environmental impacts.

## 2.9. Conclusion

In conclusion, advances in kinetic modeling of anaerobic digestion (AD) for chemical recovery in biological wastewater systems have significantly improved our understanding of the complex microbial dynamics and the biochemical processes involved in organic waste treatment. Recent developments have highlighted the need for more sophisticated and accurate models that not only predict biogas production but also optimize the recovery of valuable chemicals such as volatile fatty acids (VFAs), hydrogen, ammonia, and other bio-based products. By integrating traditional mechanistic models with data-driven approaches, such as machine learning and hybrid frameworks, researchers have been able to overcome some of the limitations of previous models, allowing for more accurate predictions and better optimization of operational parameters.

The incorporation of real-time data acquisition, model-predictive control, and digital twins represents a significant leap toward autonomous, adaptive AD systems. These advancements enable operators to fine-tune processes in real-time, making it possible to achieve higher chemical recovery rates while maintaining system stability and minimizing unwanted by-products. Furthermore, the coupling of kinetic models with microbial genomics and community dynamics has opened new avenues for understanding the specific roles of microbial species in chemical production, offering opportunities to enhance the recovery of target chemicals while optimizing microbial activity.

However, despite these advancements, there remain several challenges that must be addressed for kinetic modeling to reach its full potential in real-world applications. Data quality and availability, model overfitting, and difficulties in scaling up to diverse wastewater streams are among the primary hurdles that need further exploration. These challenges call for continued innovation in sensor technologies, computational power, and model calibration techniques. As more data becomes available and new technologies emerge, kinetic models will become increasingly reliable and better suited for predicting and optimizing chemical recovery in anaerobic digestion systems.

For the successful adoption of these models in industry, collaboration between researchers, engineers, and policymakers will be crucial. The development of standardized modeling platforms and open-access tools can enable a broader range of stakeholders to benefit from advances in AD modeling, facilitating more widespread adoption and deployment across different industries. Additionally, ongoing research into the integration of AD systems with other waste-to-resource technologies, such as microbial fuel cells or electrodialysis systems, will further expand the potential applications of AD and chemical recovery technologies.

In summary, the advances in kinetic modeling for chemical recovery in anaerobic digestion represent an exciting step forward in wastewater treatment and resource recovery. As research continues to address the challenges of data accuracy, model integration, and system scalability, kinetic modeling will play a key role in the development of more efficient, sustainable, and cost-effective AD systems. These advancements will not only improve chemical recovery but also contribute to a more circular economy, where waste is viewed as a valuable resource, helping to reduce environmental impacts while promoting sustainability in wastewater management and industrial processes.

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