Anaerobic Digestion Soft Sensor

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Anaerobic digestion is associated with various crucial variables, such as biogas yield, chemical oxygen demand, and volatile fatty acid concentration. Real-time monitoring of these variables can not only reflect the process of anaerobic digestion directly but also accelerate the efficiency of resource conversion and improve the stability of the reaction process. Therefore, it is essential to conduct soft sensor modeling for unmeasurable variables and use auxiliary variables to realize real-time monitoring, optimization, and control of the an-aerobic digestion process.

Keywords: anaerobic digestion; soft sensor; deep learning

1. Introduction

Anaerobic digestion is a highly complex biochemical reactions process, with characteristics such as multi-factor influence, dynamic change, and complex nonlinearity $^{[\underline{1}]}$. Anaerobic digestion can not only treat organic pollutants but also produce clean energy $^{[\underline{2}]}$. Therefore, anaerobic digestion technology has broad development space in the treatment of wastewater and organic solid waste $^{[\underline{3}]}$ and is one of the practical ways to solve energy and environmental problems. However, anaerobic microorganisms of the anaerobic digestion process are intensely sensitive to changes in the digestion environment, and methanogens have extremely strict requirements on the external environment $^{[\underline{3}]}$. The unexpected changes in the external environment have an impact on the hydrolysis, acidification, and methanation processes of anaerobic digestion $^{[\underline{4}][\underline{5}]}$. This will cause numerous volatile fatty acids (VFA) to accumulate in the reactor, inhibit the progress of methanation, and even result the failure of the anaerobic reactor operation $^{[\underline{6}][\underline{7}][\underline{8}]}$. Therefore, a more advanced online measurement system must be used to fully monitor the anaerobic digestion process in real-time to ensure that the anaerobic digestion process is stable and efficient while obtaining a higher biogas yield $^{[\underline{9}]}$.

In terms of anaerobic digestion process variables monitoring, there is mature and reliable online monitoring equipment for temperature, pressure, flow rate, gas composition, and other variables $\frac{[12][11]}{2}$. However, there are still many key variables that cannot be directly measured, or the measurement equipment is expensive $\frac{[12]}{2}$, such as biogas yield, chemical oxygen demand (COD), and VFA concentration. Online monitoring equipment for these variables cannot be widely used in industrial production due to factors such as expensive equipment, low accuracy, and lagging analysis $\frac{[13][14][15][16]}{2}$. Consequently, the soft sensor using online measurable auxiliary variables to estimate the unmeasurable variables in real-time has been broadly used in the anaerobic digestion process $\frac{[12][18]}{2}$. The soft sensor is developed based on the inference control theory proposed by $\frac{[19]}{2}$, suggesting that the mathematical relationship between auxiliary variables and target variables is established under certain optimal criteria, and the selection of auxiliary variables should be measurable and easy-to-obtain $\frac{[20]}{2}$. Real-time monitoring of target variables is achieved through software $\frac{[21]}{2}$. Since the soft sensor has the advantages of fast response, low cost, easy implementation, and simple maintenance $\frac{[22]}{2}$, it has been widely used in monitoring, optimization, and control of engineering $\frac{[23]}{2}$. Soft-sensor technology is broadly based on two modelling approaches: those derived mechanistically and those that are data-driven $\frac{[24]}{2}$. Specifically, mechanism models can be classified into common mechanism models and state estimation and system identification based on mechanism models $\frac{[25]}{2}$. Data-driven models can be divided into statistical machine learning models and deep learning models.

2. Anaerobic Digestion Process

2.1. Basic Principles of Anaerobic Digestion

According to the four-stage theory of anaerobic digestion proposed by Zeikus, the anaerobic digestion process can be divided into four stages: hydrolysis, acidification, acetic acidification, and methanation [26]. In the hydrolysis stage, the hydrolase hydrolyzes macromolecular organics (such as protein, fat, and cellulose) into small molecular organics (such as glucose, amino acids, and long-chain fatty acids) for subsequent reactions [26]. After the initial hydrolysis, small-molecule organic substances (such as glucose and amino acids) will be further decomposed by acid-producing bacteria to produce acidified products mainly short-chain fatty acids and secondary metabolites (such as hydrogen and carbon dioxide) [27]. In

the acetification stage, acetogens convert the organic acids and alcohols produced in the hydrolysis and acidification stages into acetic acid, generating carbon dioxide and hydrogen $\frac{[28]}{}$. In the methanation stage, acetic acid, hydrogen, and carbon dioxide are converted into methane under the action of obligate anaerobic methanogens $\frac{[29]}{}$.

2.2. Process Parameters of Anaerobic Digestion

There are some essential process variables in the anaerobic digestion process, such as pH, alkalinity, temperature, VFA concentration, COD, and biogas yield. Real-time monitoring of the above variables can ensure the efficient and stable operation of the anaerobic digestion process. However, there is little widely used real-time monitoring equipment for VFA concentration, COD, and biogas yield.

- PH: The optimal pH range of different microorganisms is different. Methanogens are extremely sensitive to pH, and the optimal pH range is 6.5–7.2 [30]. The fermenting microorganisms produce acetic acid and butyric acid when the pH is low. Acetic acid and propionic acid are formed when the pH is higher than 8.0 [31]. Therefore, reasonable monitoring of pH can ensure the maximum biological activity of microorganisms.
- Alkalinity: Methanogens usually produce alkalinity in the form of carbon dioxide, ammonia, and bicarbonate, contributing to neutralizing VFA produced during anaerobic digestion [32]. Thus, real-time monitoring of alkalinity can improve the stability of the anaerobic digestion process when the concentration of carbon dioxide is stable.
- Temperature: Temperature has a crucial influence on the physical and chemical properties of anaerobic digestion and fermentation substrates. It affects the growth rate and metabolism of microorganisms, which in turn influences the population dynamics of the anaerobic digestion process [33]. When the temperature changes more than 1 °C/day, the biochemical activity of methanogens will be severely affected, causing the process to fail.
- VFA concentration: VFA concentration is an intermediate product of the anaerobic digestion process. Excessive accumulation of VFA can reduce the pH of the system and inhibit the activity of methanogens. The VFA concentration can reflect the current operating conditions of the system while being extremely sensitive to the incoming feed imbalance [34]. Hence, it is urgent to establish a soft sensor to predict the VFA concentration by monitoring the measurable and easy-to-obtain process variables in real-time.
- COD and biogas yield: COD is an imperative indicator to measure the organic content of the effluent from the
 anaerobic digestion process [35]. Biogas yield is a vital indicator to measure the efficiency of anaerobic digestion [36].
 Real-time monitoring of COD and biogas yield can demonstrate the operating efficiency and stability of the anaerobic
 digestion process and contribute to achieving the real-time calibration and optimization of production conditions and
 control methods.

2.3. Anaerobic Digestion Process

In the industrial production process, anaerobic digestion processes are usually classified according to factors such as operating temperature, feeding method, and the number of reactors $\frac{[3Z]}{2}$. It can be divided into single-phase digestion and two-phase digestion based on the number of reactors $\frac{[3B]}{2}$. The single-phase digestion process was widely used in the immature stage of the early anaerobic digestion theory due to its low price and simple operation. Single-phase digestion suggests that the hydrolysis, acidification, acetic acidification, and methanation processes of degrading macromolecular organics are all conducted in the same digestion tank, and the inhibition of any one step will affect the overall digestion efficiency $\frac{[39]}{2}$. With the development of the anaerobic digestion theory, researchers and technologists have developed a two-phase digestion process to avoid acid inhibition. Two-phase anaerobic digestion suggests the hydrolysis, acidification, and acetic acid stages are conducted in the acid production tank, while the methane production stage is performed in the methane production tank $\frac{[40]}{2}$. This method can effectively avoid mutual inhibition between the steps, improve the efficiency of anaerobic digestion, shorten the reaction time, and increase methane production $\frac{[41]}{2}$.

According to the biodegradability of the input materials, different two-phase anaerobic digestion devices are generally selected $^{[42]}$. When industrial wastewater is treated with low solid content, the acid production tank and the methane production tank usually adopt a continuous stirred tank reactor and an up-flow anaerobic sludge blanket, respectively $^{[43]}$. When organic wastewater is treated with high solid content, both the acid production tank and the methane production tank use the up-flow solid reactor $^{[44]}$. When organic sludge is processed with higher solid content, both the acid production tank and the methane production tank employ the continuous stirred tank reactor $^{[45]}$. The specific process flow is described as follows $^{[28]}$. First, the pretreated organic materials are fed into the hydrolysis acidification tank to perform the hydrolysis reaction of macromolecular organics and the acidification reaction of small molecular organics. Then, the acidified product is input into the methane-generating tank for methane production reaction. Since the stages of acid

production and methane production are performed separately, it is ensured that acid-producing bacteria and methanogens are in optimal environmental conditions and can exert maximum activity. Moreover, the acid production process improves the biochemical properties of the material, and the acidified product provides a suitable substrate for methanogens. The two-phase anaerobic digestion process is illustrated in **Figure 1**.

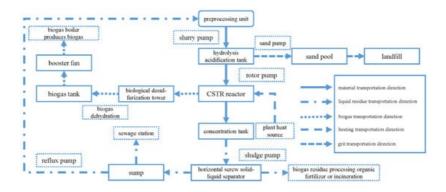


Figure 1. Two-phase anaerobic digestion process flow chart.

3. The Latest Development of Anaerobic Digestion Soft Sensor

The previous chapter introduced traditional anaerobic digestion soft sensors, reflecting the mapping relationship between auxiliary variables and target parameters to a certain extent. The characteristics of traditional soft sensors are summarized in **Table 1**. However, soft sensors still face many challenges in practical applications. For example:

Table 1. Advantages and disadvantages of traditional soft sensors.

| Soft Sensors | Advantages of Soft Sensor | Defects of Soft Sensor |
|---|---|--|
| Soft sensor based on process mechanism | High precision, strong interpretability, clear industrial background | It is difficult to build an accurate mechanism model |
| Soft sensor based on state estimation | Solve the problem of dynamic characteristic differences and system lag between variables | Simplifying the system will increase forecast errors |
| Soft sensor based on MLR | Only consider the mapping relationship of data; do not require a clear internal mechanism | The accuracy is not high, and it is easily affected by external interference |
| Soft sensor based on PLSR | Solve the problem of collinearity between auxiliary variables | Inability to handle strong nonlinear problems |
| Soft sensor based on BP neural network | Able to achieve an arbitrary precision approximation of nonlinear functions | Easy to fall into local optimal or over- fitting state |
| Soft sensor based on RBF neural network | Realize the global best approximation and solve the local optimal problem | Affected by network topology and hyperparameters |
| Soft sensor based on SVR | Solve the problem of high dimensions and small samples | Unable to handle large-scale data |
| Soft sensor based on LS-SVR | Further reduce the complexity of the model and increase the calculation speed | Very sensitive to outliers and poor robustness |

• The traditional soft sensor cannot extract the deep features of auxiliary variables. The performance of traditional soft sensors depends on the auxiliary variables provided, and the selection of auxiliary variables requires rich prior knowledge [46].

- The traditional soft sensor does not consider the large number of unlabeled samples in the anaerobic digestion process. There are many unlabeled samples in the anaerobic digestion process. The semi-supervised learning mechanism, which is used to mine unlabeled sample information, can effectively improve the prediction performance of soft sensors [47].
- The traditional soft sensor does not consider the dynamic and time lag characteristics of anaerobic digestion. The traditional soft sensor cannot adapt to changes in work and production conditions, and the prediction accuracy of the soft sensor gradually deteriorates over time [48]. Meanwhile, the slow hydrolysis process of anaerobic digestion would lead to a certain time lag between the real-time monitoring variables of the acid-producing tank and the real-time monitoring variables of the methane-producing tank.
- The traditional soft sensor only considers the mapping relationship between auxiliary variables and target variables while ignoring the mutual influence between auxiliary variables [49]. In the actual industry, the combined auxiliary variables are generally highly correlated with the target variable while the single auxiliary variable often has a weak correlation with the target variable.

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