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Dynamic model reduction for two-stage anaerobic digestion processes

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HIGHLIGHTS

- Modeling of two-stage anaerobic digestion is studied and compared to one-stage.
- Two-stage operation could lead to higher product purity under optimal conditions.
- Two-stage operation could not lead to significant enlargement of stability region.
- Invariant manifold methods and observability analysis are used for model reduction.
- Reduced model is of only 3rd order, but in excellent agreement with original model.

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ABSTRACT

This paper deals with the development, analysis and reduction of a two-stage anaerobic digestion process model. A two-stage model based on a two-step mass-balance model is first developed. The model incorporates two stages as two similar CSTRs, with acidogenesis in the first stage and mainly methanogenesis in the second. Steady state optimization validates the benefits of two-stage operation compared to the traditional one-stage process. Using reaction invariants, the dynamics of the fast modes is neglected by projecting the overall system dynamics on the slow-motion invariant manifold, and the original 7-state model is reduced to a 5th order system. By neglecting the nearly unobservable modes, the model is further reduced to 3rd order. Simulation results show excellent accuracy of the reduced model compared to the detailed one. At the same time, they indicate the necessity of process control for stabilization of the system.

1. Introduction

Production of methane via anaerobic digestion of biogenic material is an alternative renewable energy source. Among various methods for energy production from biomass (e.g. bioethanol, pyrolysis, biodiesel, etc.), anaerobic digestion has shown to be a robust, cheap and independent process. It can run on a wide variety of substrates, contributes to carbon and methane capture, does not require a sterile process, can be very stable under conservative operation, has minimal safety requirements, and the digestate may be used as fertilizer. Still, with the process being carried out by a large symbiotic and constantly changing microbial population (mainly due to mutations, non-sterile feeding, and low dilution rates), and with the sludge making state monitoring costly and maintenance-intensive, there are major challenges in the dynamic operation and control of the process. This has led to conservative operation strategies, far from optimal yields and lacking the necessary flexibility to comply with fluctuations in both feed and demand.

The anaerobic digestion process involves four main biochemical steps, namely: 1) hydrolysis, 2) acidogenesis, 3) acetogenesis, and 4) methanogenesis. These steps are carried out by different microbial populations with varying characteristics, growth rates and substrate affinities. Most anaerobic digestion processes run in a single stage limiting the operation to a single dilution rate. Nevertheless, there is a set of optimal dilution rates for each population, so that dividing the process in different reactors could be advantageous. Pohland [1] proposes to run the process in two different reactors promoting hydrolysis/acidification in the first reactor and acetogenesis/methanogenesis in the second one. By this, different groups of microorganisms (hence steps of the process) are divided into separate reactors that run at their respective optimal operating conditions. As a result, increased production rate, higher product purity and improved process stability may be expected. A number of experimental studies supporting this idea have been

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published [2,3,4,5]. Therefore, there is significant motivation for modeling and analysis of the two-stage process, for the purpose of optimal design and operation.

An inherent property of anaerobic digestion processes is that they are self-regulatory at low dilution rates. However, in order to improve the methane production rate per volume, high dilution rates are necessary, in which case there is an increased risk of washout caused by process disturbances. For this reason, process control is of major significance in anaerobic digestion processes in terms of stabilizing the process, as indicated by the large number of publications dealing with control of the one stage process (see e.g. [6–12]).

In order to be able to develop a successful two-reactor anaerobic digestion technology, it is important to build accurate mathematical models for each stage. There have already been a variety of established models to describe the traditional one-stage process [12–15]. The Anaerobic Digestion Model No.1 (ADM1) is rather complicated but proved to be fairly accurate in describing a number of important anaerobic digestion processes. Other models, like the one in [13], are more concise and more suitable for control purposes. For the two-stage process, one can easily derive a dynamic model by applying the one-stage model twice [16,17], but there is a question of whether doubling the dimension of the system would be necessary to adequately describe the process dynamics. Thus, it would be meaningful to explore the prospect of reducing the system dimensionality. For a one-stage process, reduction of model dimensionality has been studied in the literature. There are some numerical methods, like using balancing of empirical gramians [18] and methodology based on PCA [19], showing the capability of simplifying complicated models like ADM1. The invariant manifold approach [20] based on the fact that the acidogenic bacteria growth rate is much faster than that of methanogens, gives an analytical procedure to reduce the model in terms of the physical variables and parameters of the system. It would be important to investigate whether similar rigorous principles could be applied on the two-stage process.

The present work has two goals. First, to set up a mathematical model for a two-stage process based on the model of [13] for each stage, and to explore the advantages (in terms of its optimality characteristics) as well as the challenges (in terms of its narrow stability region) of two-stage anaerobic digestion. Second, and more important, to reduce the complexity of the dynamic model for the two-stage process using rigorous mathematical methods. The reduced dynamic model will be significantly simpler than the original one, while retaining the same accuracy of the original model, in terms of predicting its static and dynamic characteristics.

Section 2 will first provide a brief necessary review of the model in [13] for a one-stage anaerobic digestion process, which will be subsequently used to develop a detailed dynamic model for the two-stage process. This detailed model will be used to calculate the optimal operating conditions for the two-stage process and compare them to the ones of one-stage process in terms of production rate and purity of biogas. In addition, the challenges of optimal operation (in either one-stage or two-stage case) will be explored, in terms of the severely limited stability region.

Section 3 will define the model reduction problem. It will explicitly state the assumptions involved and discuss both the steady state and eigenvalue characteristics of the system, which will play a critical role in the derivation of the reduced model.

Section 4 will provide a brief necessary review of the invariant manifold method for dynamic systems involving two different time scales.

Section 5 will include the main mathematical derivation of the present paper. Model reduction will be initially achieved by eliminating the fast modes via projection of the dynamics on the slow motion invariant manifold, and further reduction will be achieved by eliminating nearly unobservable modes of the system.

Section 6 will evaluate the accuracy of the derived reduced model through a simulation study. Time responses as well as phase portraits for detailed and reduced models will be compared and evaluated. The results will indicate the excellent accuracy of the reduced model and at the same time will motivate the need for process control, which will be studied in a future paper.

2. One-stage versus two-stage operation in biogas production

There are various alternative dynamic models describing the anaerobic digestion process. But for control purposes, complex models are difficult to use. More specifically, for the purpose of developing a monitoring and control system for two-stage anaerobic digestion processes, a good starting point is the model proposed by Bernard et al. [13], which involves lumping to reduce model complexity. This can be further reduced, as will be seen in the next sections.

2.1. Dynamic model for one-stage anaerobic digestion process [13]

In this model, it is assumed that anaerobic digestion is a two-step process, as is indicated in Fig. 1, and all the bacterial populations are categorized into two different groups with homogeneous characteristics. In the acidogenesis step, the organic substrate (S_1) is consumed by acidogenic bacteria (X_1), with volatile fatty acids (VFAs, S_2) and CO_2 as products. In the subsequent methanogenesis step, the population of methanogenic bacteria (X_2) grows with the consumption of VFAs, to produce CO_2 and methane gases. The mass-balance model for the CSTR is

$$
\begin{aligned}
\frac{dX_1}{dt} &= D\cdot(X_1^0 - X_1) + Y_1\cdot\mu_1(S_1)\cdot X_1\\
\frac{dX_2}{dt} &= D\cdot(X_2^0 - X_2) + Y_2\cdot\mu_2(S_2)\cdot X_2\\
\frac{dS_1}{dt} &= D\cdot(S_1^0 - S_1) - \mu_1(S_1)\cdot X_1\\
\frac{dS_2}{dt} &= D\cdot(S_2^0 - S_2) + c\cdot\mu_1(S_1)\cdot X_1 - \mu_2(S_2)\cdot X_2\\
\frac{dZ}{dt} &= D\cdot(Z^0 - Z)\\
\frac{dC}{dt} &= D\cdot(C^0 - C) - q_c(S_2,Z,C) + Y_3\cdot\mu_1(S_1)\cdot X_1 + Y_4\cdot\mu_2(S_2)\cdot X_2
\end{aligned}
\tag{1}
$$

In addition to X_1, X_2, S_1 and S_2 defined before, the model contains two more states, the total alkalinity Z and the total inorganic carbon in water C, which is mainly composed of dissolved CO_2, bicarbonate and carbonate.

X_1^0, X_2^0, S_1^0, S_2^0, C^0 and Z^0 are the inlet concentrations of X_1, X_2, S_1, S_2, C and Z, respectively, and $D = F/V$ is the dilution rate. μ_1 and μ_2 (d^{-1}) represent the specific growth rate of the two groups of bacteria, which can be described as follows:

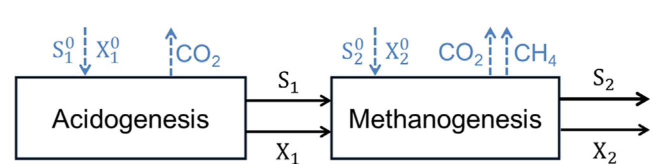

Fig. 1. One-stage anaerobic digestion process (Solid arrows refer to states of the model and dash arrows refer to inlet and gas-phase outlet flow of the physical system).