UNIVERSIDAD TÉCNICA FEDERICO SANTA MARIA

DEPARTAMENTO DE ELECTRÓNICA

VALPARAISO - CHILE

"State Estimation and Model Predictive Control of the Anaerobic Digestion Process for the Optimization of Biogas Production"

MICHEL ANDRÉS AZÚA POBLETE

Thesis Submitted in Partial Fulfillment of the Requirements for the Degree of Master of Science in Electronic Engineering

THESIS ADVISOR: DR. JUAN CARLOS AGÜERO
CO-ADVISOR: DR. ANGEL CEDEÑO
CO-ADVISOR: DR. SANTIAGO GARCIA

SEPTEMBER 2025

CONSTANCIA DE VALIDACIÓN Y CONFIDENCIALIDAD DE MONOGRAFÍA A REPOSITORIO ACADÉMICO

1.- IDENTIFICACIÓN DEL TRABAJO ACADÉMICO

Tipo de monografía (marcar una opción): ☐ Memoria o trabajo de título; ☒ Tesis de Postgrado;

Título del trabajo: State Estimation and Model Predictive Control of the Anaerobic Digestion Process for the Optimization of Biogas Production

Nombre del candidato(a): Michel Andrés Azúa Poblete

Carrera / Grado: Magister en las Ciencias de la Electrónica

Campus: Casa Central Valparaiso ; **Departamento**: Electronica

2.- VALIDACIÓN DEL PROFESOR GUÍA/DIRECTOR DE TESIS

Yo, Juan. C Agüero, en mi calidad de profesor(a) guía/director(a) del trabajo académico mencionado anteriormente **DEJO CONSTANCIA** que:

- He revisado esta versión del documento y corresponde a la versión final aprobada del trabajo.
- El trabajo cumple con los requisitos académicos y de formato establecidos por la institución

3.- EVALUACIÓN DE CONFIDENCIALIDAD POR PROPIEDAD INDUSTRIAL

☐ El trabajo **NO contiene información que amerite confidencialidad** y puede ser publicado de inmediato en repositorio con acceso abierto.

☒ El trabajo **CONTIENE** información con potenciales implicancias de propiedad industrial o intelectual y requiere un periodo de confidencialidad (embargo) por:

☒ 6 meses; ☐ 12 meses; ☐ 2 años; ☐ 3 años; ☐ 5 años; ☐ 10 años

Fundamentación de la necesidad de confidencialidad (obligatorio si se solicita embargo):
Se encuentra un paper asociado al tema de tesis en espera de aprobación de publicacion en una revista cientifica.

4.- FIRMAS

Profesor(a) guía o director(a) de memoria o tesis:

Fecha: 01/09/2025 ; **Firma:** ____________________

Estudiante o Candidato(a):

Fecha: 01/09/2025 ; **Firma:** ____________________

Este formulario debe ser insertado como página 2 de la memoria o tesis, completado y firmado por estudiante y profesor(a) antes de la entrega en portal PRISMA de Biblioteca USM.

BIB-FO2385 01

Acknowledgements

I thank my family, especially my mother, father, and Tony, whose unwavering support has been indispensable for my personal development in every aspect of my life. The foundation they provided has been crucial to my university journey, and I owe them everything.

I am deeply grateful to my professors and teaching assistants, whose wisdom and precise knowledge have shaped my education. Their patience, professionalism, and dedication have been invaluable. Wherever my professional path may lead, I will carry their teachings with me. Thank you for your perseverance and tolerance in sharing your expertise.

I also want to thank GOTH, who accompanied me throughout my entire time of study, offering invaluable companionship and support during the most challenging moments.

Finally, I would like to express my heartfelt gratitude to the WBI Service Bourse of Wallonie-Bruxelles International for their financial and research support, which made my research residency possible.

DEPARTAMENTO DE ELECTRONICA
UNIVERSIDAD TECNICA FEDERICO SANTA MARIA

Estimación de estados y control predictivo del proceso de digestión anaerobia para la optimización de la producción de biogás

Michel Andrés Azúa Poblete

Tesis para optar al título de Magister en las Ciencias de la Ingeniería Electrónica.

Universidad Técnica Federico Santa María

Profesor Guía: Dr. Juan Carlos Agüero

September 2025

Resumen

Esta tesis se centra en la optimización del proceso de digestión anaeróbica (DA). Se desarrolló un modelo matemático discreto (AM2), inspirado en el modelo ADM1, para representar de manera precisa las dinámicas específicas del proceso en estudio. Este modelo fue calibrado y validado utilizando datos simulados obtenidos del modelo ADM1. Mediante la implementación de un control predictivo no lineal (NMPC) y un filtro de Kalman extendido (EKF), se logró controlar y optimizar significativamente el desempeño del proceso con el objetivo de maximizar la producción de biogás. Esta investigación contribuye al avance en el control de procesos químicos, ofreciendo herramientas valiosas para aplicaciones industriales y ambientales.

Keywords: *NMPC*, *EKF*, *Digestion Anaerobica*, *Observadores*, *Identificación de parámetros*, *Acción Integral*.

State Estimation and Predictive Control of the Anaerobic Digestion Process for Biogas Production Optimization

Michel Andrés Azúa Poblete

Thesis for the Master's Degree in Electronic Engineering

Universidad Técnica Federico Santa María

Advisor: Juan Carlos Agüero, PhD.

September 2025

Abstract

This thesis focuses on the optimization of the anaerobic digestion (AD) process. A discrete mathematical model (AM2), inspired by the ADM1 model, was developed to accurately represent the specific dynamics of the process under study. This model was calibrated and validated using simulated data obtained from the ADM1 model. By implementing a nonlinear predictive control (NMPC) and an extended Kalman filter (EKF), it was possible to significantly control and optimize the performance of the process with the objective of maximizing biogas production. This research contributes to the advancement of chemical process control, offering valuable tools for industrial and environmental applications.

Keywords: *NMPC*, *EKF*, *Anaerobic Digestion*, *Observers*, *Parameter Identification*, *Integral Action.*

Contents

List of Tables

List of Figures

1. Introduction

The management and treatment of organic waste represent a crucial challenge in the context of sustainability and environmental protection. As the global population continues to grow, the amount of organic waste produced increases significantly, necessitating effective waste management strategies to mitigate environmental impact. Among the technologies developed to address this challenge, Anaerobic Digestion (AD) stands out for its efficiency and sustainability. This biological process transforms organic matter into biogas in the absence of oxygen, contributing both to waste reduction and the generation of renewable energy. Biogas, primarily composed of methane (CH_4) and carbon dioxide (CO_2), can be used to produce electrical and thermal energy, thus promoting energy sustainability [1–3].

AD involves the decomposition of organic matter by microorganisms under anaerobic conditions, producing both biogas and a stabilized digestate, which can be used as fertilizer. This technology has evolved from the use of septic tanks to high-rate digesters and co-digestion (CoDA), which allows for the simultaneous treatment of various types of waste, offering environmental, technological, and economic benefits [4]. CoDA, in particular, enhances biogas production by optimizing nutrient ratios and improving microbial activity, thus further contributing to the overall efficiency of waste treatment processes.

Despite these advancements, the efficiency of the AD process can be affected by the variability in waste composition and the operational conditions of the digester. Factors such as temperature, pH, and the presence of inhibitors can significantly influence microbial performance, leading to fluctuations in biogas yield and composition. Conventional control methods, such as PID controllers, often prove insufficient for managing the complexity and nonlinearity of the process [5]. These methods typically rely on linear assumptions that do not adequately capture the dynamic behavior of anaerobic digestion, resulting in suboptimal performance and potential operational issues.

Therefore, there is a need to apply advanced control techniques to optimize the performance of the process. Model Predictive Control (MPC) has been widely used for managing complex processes across various industries, offering the ability to predict future system behavior and optimize control actions accordingly. However, its application in nonlinear and stochastic systems, such as anaerobic digestion, presents significant challenges. In this context, Nonlinear Model Predictive Control (NMPC) emerges as a promising solution. NMPC allows for managing systems with constraints and complex dynamics, adjusting control actions based on future predictions of the system [6]. This technique provides more precise and adaptive optimization by handling the inherent nonlinearity and uncertainties of the system.

In summary, the integration of NMPC in the control of anaerobic digestion processes offers a pathway to enhance efficiency, stability, and adaptability in the management of organic waste. This thesis aims to explore the potential of NMPC combined with advanced estimation techniques, such as Extended Kalman Filters (EKF), to develop a robust control strategy that addresses the challenges of anaerobic digestion. By improving control accuracy and reducing steady-state errors, this research seeks to contribute to the advancement of sustainable waste management practices and the optimization of renewable energy production.

1.1. State of the Art

In the field of anaerobic digestion (AD) control, various strategies have been implemented to improve process efficiency. Traditional approaches, such as Proportional-Integral-Derivative (PID) controllers, have proven inadequate for addressing the inherent complexity of biological systems [7]. PID controllers typically rely on linear assumptions and fixed parameters, which do not account for the dynamic and nonlinear behavior of AD processes. This limitation can lead to suboptimal performance, especially in the face of varying feedstock compositions and operational conditions.

The introduction of Model Predictive Control (MPC) has provided significant improvements in process regulation, allowing for more sophisticated management of system dynamics. MPC uses a dynamic model of the process to predict future behavior and optimize control actions accordingly, which makes it well-suited for managing complex systems. However, the adaptation of Nonlinear Model Predictive Control (NMPC) to AD is still under development and faces specific challenges.

Dynamic models of AD and co-digestion (CoDA) have been fundamental in understanding process behavior and evaluating the viability of different waste mixtures [8, 9]. These models allow for the simulation and analysis of process evolution, providing insights into the interactions between various parameters. Nevertheless, the effective implementation of NMPC in this context requires a more refined approach, especially regarding state estimation in nonlinear and stochastic systems. The reliance on accurate models is critical for making informed control decisions, as inaccuracies can propagate through the system and lead to inefficiencies or instability.

Despite advances in anaerobic digestion control, significant challenges remain, including:

- **Model Complexity:** The nonlinear and stochastic nature of the AD process presents a challenge for the effective application of NMPC. Developing an accurate model that properly reflects process dynamics is essential for the successful implementation of NMPC [10–12]. This involves not only capturing the biological reactions and interactions among microorganisms but also accounting for variations in feedstock composition and environmental conditions. Researchers are exploring various modeling approaches, including mechanistic and data-driven models, to enhance the accuracy and robustness of AD simulations.

- **State Estimation:** Obtaining accurate real-time measurements is costly and complicated due to the inherent variability of the process. Advanced estimation techniques, such as the Extended Kalman Filter (EKF) [13, 14] and Particle Filter (PF) [15, 16], play a crucial role in improving state estimation accuracy and control reliability. These techniques enable the assimilation of noisy measurements and the prediction of unobservable states, allowing for more informed control actions. The integration of state estimation with NMPC is essential for addressing uncertainties and enhancing overall system performance.

- **Process Optimization:** Implementing an NMPC control scheme specifically adapted for AD can significantly improve process optimization. This involves adjusting control actions based on future predictions and effectively managing system constraints, allowing for more stable and efficient process management [17–20]. Key aspects of optimization include maintaining optimal conditions for microbial activity, minimizing variations in biogas production, and ensuring the stability of the digester operation. Successful implementation of NMPC requires careful consideration of trade-offs between competing objectives, such as maximizing biogas yield and minimizing operational costs.

Although advances in control and modeling technology have improved anaerobic digestion management, the application of NMPC still faces significant challenges. Integrating advanced techniques for state estimation and process optimization is crucial for overcoming these challenges and achieving more effective and sustainable AD management. Future research should focus on developing robust models, enhancing estimation techniques, and refining NMPC algorithms to better address the complexities of anaerobic digestion systems.

1.2. Objectives

The work focuses on two main objectives aimed at improving the efficiency of the anaerobic digestion process through the use of advanced control and estimation techniques.

- **Development of a Nonlinear Filtering Algorithm:** The first objective is to develop a nonlinear filtering algorithm to estimate the variables of the anaerobic digestion process. This will involve gathering information from previous research on the discrete AM2 model and applying the corresponding filtering algorithms. In cases where only continuous models are available, discretization techniques will be employed to adapt these models. The Extended Kalman Filter (EKF) and Particle Filter (PF) will be primarily evaluated to perform estimations of the nonlinear AM2 model. These algorithms will enhance the accuracy of state estimations, which is crucial for effective process management.

- **Development of a Nonlinear Model Predictive Controller (NMPC):** The second objective involves developing a predictive controller to optimize the anaerobic digestion process. This includes identifying and measuring multiple process variables, accurately configuring the control algorithms, and integrating the controller with the digital twin of the process. The predictive controller will adjust control actions based on future predictions of the system, optimizing biogas production, digestate quality, and system stability.

- **Process Optimization with NMPC Integration:** The primary goal of the project is to enhance the efficiency of the ADM1 process using the AM2 model to make predictions and obtain optimal control signals through the MPC controller. It builds upon an NMPC algorithm developed in the referenced work [21]. The expectation is that the implementation of the MPC approach with integration will be more effective and produce better results in optimizing the biogas production process through anaerobic digestion.

Based on the description above, the following specific objectives are defined:

- Develop a precise and efficient discrete mathematical model of the anaerobic digestion process that incorporates fermentable soluble substrates, allowing reliable and accurate simulation of the process.
- Estimate key states of the anaerobic digestion process using nonlinear filtering algorithms to improve model accuracy and validate its performance under various operating conditions.
- Implement a predictive controller based on the mathematical model to optimize the anaerobic digestion process in terms of methane production, digestate quality, and system stability.

1.3. Hypothesis

The hypothesis is that it is possible to develop an effective method for controlling and estimating the states of an anaerobic digestion process using nonlinear predictive control techniques and filtering algorithms. It is expected that validation through simulations will show a significant improvement in process performance, optimizing biogas production and system stability, and providing a solid foundation for implementation in real-world environments.

This hypothesis underscores the potential of advanced control methodologies to enhance the management of anaerobic digestion processes, suggesting that the integration of NMPC and nonlinear filtering can effectively address the challenges posed by the nonlinear and variable nature of the system. By validating this hypothesis, the research aims to contribute valuable insights and tools for optimizing biogas production and improving the overall efficiency of anaerobic digestion systems.

1.4. Publications Related to the Thesis Work

1. Scientific Journal:

    - M. Azúa-Poblete, A. L. Cedeño, J. C. Agüero, Linio O. Santos, Laurent Dewasme, Alain Vande Wouwer and S. García-Gen. "Enhancing Anaerobic Digestion Performance With Offset-Free Model Predictive Control", 2025 (Submitted to a journal).

      Abstract: This study focuses on the development of a nonlinear model predictive controller of an anaerobic digestion process acting on the dilution rate so as to track a target methane flow rate. Nonlinear model predictive control uses a predictor based on a simplified two-stage anaerobic digestion model, and an extended Kalman filter to estimate the system states and a disturbance state, which mostly represents the prediction bias of the model. The estimation of the disturbance state introduces an integral action to the nonlinear model predictive control strategy and provides offset-free performance even when the simplified model is unable to predict the real system state accurately. The algorithm was successfully tested in a simulation environment with readily biodegradable soluble wastes, using the *Anaerobic Digestion Model No. 1* as a plant emulator. The integral action and disturbance state estimation are critical to the controller performance.

2. Conference:

    - M. Azúa-Poblete, A. L. Cedeño, S. García-Gen and J. C. Agüero, "On State Estimation Methods for an Anaerobic Digestion Model for Readily Biodegradable Substrates," 2023 IEEE CHILEAN Conference on Electrical, Electronics Engineering, Information and Communication Technologies (CHILECON), Valdivia, Chile, 2023, pp. 1-6, doi: 10.1109/CHILECON60335.2023.10418604.

      Abstract: This paper focuses on the state estimation of an Anaerobic Digestion (AD) model using two filtering algorithms: the Extended Kalman Filter (EKF) and the Particle Filter (PF). AD is a biological process converting organic matter into biogas, offering both a valuable renewable energy source and a sustainable solution for waste treatment. We investigate the applicability of these methods to the state space model called AM2, a simplified AD model involving only the key acetogenesis and methanogenesis reactions and excluding other specific biochemical steps. Subsequently, we evaluate their performance through simulation experiments.

1.5. Thesis Structure

This thesis will be divided into the following sections:

- **Chapter 2: Concepts.**

  This chapter will detail the advanced control techniques that were implemented in this thesis. These techniques are presented beforehand to facilitate understanding of the results without interrupting the reading flow.

- **Chapter 3: Problem Statement.**

  This chapter will describe the plant of interest to be controlled. Existing models and previous results will be detailed, as this work is a continuation of a previous thesis.

- **Chapter 4: Problem Resolution.**

  This chapter will present how the various control techniques detailed in Chapter 2 were implemented to control the anaerobic digestion plant.

- **Chapter 5: Results.**

  This chapter will present the results obtained from implementing the various control strategies developed in this thesis. An analysis will be performed using metrics to determine the best control strategy.

- **Chapter 6: Conclusions.**

  This chapter will discuss the results obtained in this thesis and comment on possible future work.

2. Concepts

This section will detail some concepts that will be fundamental for addressing the problem posed in this thesis.

2.1. Filtering Algorithm

A filtering algorithm is a technique used in control theory and statistics to estimate the state of a dynamic system in real time. Its purpose is to obtain accurate estimates of the state, even with incomplete or noisy measurements. Filtering is essential in signal processing and control systems, where it is crucial to obtain precise measurements of variables that may not be directly observable or may be contaminated with noise. This noise can originate from various sources, such as unknown inputs, noisy sensors, or noisy transmission channels.

The goal of filtering is to recover a quantity of interest, denoted as $\hat{x}(t)$, from noisy measurements $y(t)$ and $u(t)$, when they are available. Filtering is used to distinguish a certain type of information processing from two related types: filtering, prediction and smoothing. In this context, filtering means recovering information about $\hat{x}(t)$ at time t using measurements up to time t.

When implementing control systems, the signals u_t and y_t are often known through sensors in the control system, but the states x_t are usually not directly accessible or economically viable to measure. An alternative in such cases is to obtain an estimate of these states through a state observer.

One of the most widely used algorithms for state estimation is the Kalman Filter (KF), which provides optimal performance in linear systems subject to Gaussian noise. For nonlinear systems, extensions such as the Extended Kalman Filter (EKF) and the Unscented Kalman Filter (UKF) are employed. These variants incorporate both the system's dynamics and noisy measurements to iteratively update and refine state estimates. Specifically, the EKF linearizes the nonlinear system around the current estimate, allowing Kalman Filter principles to be applied in scenarios where strict linearity does not hold.

Filtering techniques are fundamental in real-time applications such as robotics, aerospace, and industrial automation, where accurate state estimation directly impacts system performance and safety. For instance, autonomous vehicles use filters to estimate position and velocity from noisy sensor data (e.g., GPS, accelerometers, gyroscopes). In aerospace, filters contribute to attitude and velocity estimation for aircraft and spacecraft. Likewise, in chemical and biological processes, filters enable precise control even when sensor data is noisy, delayed, or sparse.

Filtering is also critical in adaptive control systems, where model parameters or system dynamics may vary over time. In such contexts, a reliable filter enhances controller performance by providing accurate and updated state estimates, increasing robustness and adaptability.

In cases involving non-Gaussian noise or strongly nonlinear dynamics, more advanced techniques like Particle Filters (PF) are used. PF approximate the probability distribution of the state using a set of weighted samples (particles), offering greater flexibility in representing complex systems.

In summary, filtering is a key component of modern control strategies. It enhances real-time state estimation, supports robust decision-making, and improves overall system performance under uncertainty.

The following section presents the filtering algorithm employed in this thesis.

2.1.1. Kalman Filter

The standard Kalman filter [22] is one of the most recognized and widely used filtering algorithms in the literature. This filter has been applied in a variety of contexts where the system is linear (for both states and outputs) and the associated noises are Gaussian. This algorithm addresses a linear system characterized by the following equations:

$$x_{t+1} = Ax_t + Bu_t + w_t, \tag{2.1}$$

$$y_t = Cx_t + Du_t + v_t, \tag{2.2}$$

where A, B, C, and D are matrices that define the dynamics of the model, while w_t and v_t

represent uncorrelated Gaussian noise. It is assumed that the signals y_t, u_t and x_1 are known.

The filtering equations provide a closed-form solution expressed as follows:

$$p(x_1) = \mathcal{N}\left(x_1; \mu_1, \Sigma_1\right), \tag{2.3}$$

$$p(x_t|y_{1:t}) \approx \mathcal{N}\left(x_t; \hat{x}_{t|t}, \Sigma_{t|t}\right), \tag{2.4}$$

$$p(x_{t+1}|y_{1:t}) \approx \mathcal{N}\left(x_{t+1}; \hat{x}_{t+1|t}, \Sigma_{t+1|t}\right), \tag{2.5}$$

where $p(x_1)$ denotes the initial distribution of the state x_1, $p(x_t|y_{1:t})$ indicates the posterior distribution of the state x_t given all measurements up to time t, and $p(x_{t+1}|y_{1:t})$ represents the predictive distribution of the state x_{t+1} given all measurements up to time t.

The equations for the Kalman Filter (KF) are articulated as follows:

$$K_t = \Sigma_{t|t-1} C_t^T (R + C_t \Sigma_{t|t-1} C_t^T)^{-1}, \tag{2.6}$$

$$\hat{x}_{t|t} = \hat{x}_{t|t-1} + K_t\left(y_t - C\hat{x}_{t|t-1} - Du_t\right), \tag{2.7}$$

$$\Sigma_{t|t} = (I - K_t C)\Sigma_{t|t-1}, \tag{2.8}$$

$$\hat{x}_{t+1|t} = A\hat{x}_{t|t} + Bu_t, \tag{2.9}$$

$$\Sigma_{t+1|t} = Q + A\Sigma_{t|t}A^T, \tag{2.10}$$

with initialization parameters set as $\hat{x}_{1|0} = \mu_1$ and $\Sigma_{1|0} = \Sigma_1$.

The Kalman filter operates through two primary phases: prediction and correction, which work together to provide optimal state estimates in dynamic systems.

During the prediction phase, the filter utilizes the system's state transition model to project the current state estimate forward in time. This involves calculating a predicted state based on the previous estimate and the system dynamics.

After the prediction phase, the correction phase integrates new measurements to refine the predicted state estimate. This is achieved by updating the predicted state with a weighted difference between the actual measurement and the predicted measurement. By incorporating this new measurement, the correction phase adjusts the predicted state, thereby enhancing the accuracy of the state estimate.

This two steps process—prediction followed by correction enables the Kalman filter to effectively estimate the state of dynamic systems, even in the presence of noise and uncertainty.

2.1.2. Extended Kalman Filter

The Extended Kalman Filter (EKF) is an extension of the Kalman Filter designed to estimate nonlinear systems by applying local linearization around the currently estimated state. This filter combines the predictions from the nonlinear model with current measurements using the equations of the Kalman Filter to obtain an sub-optimal estimate of the system state.

Considering a nonlinear system of the form:

$$x_{t+1} = f(x_t, u_t) + w_t, \tag{2.11}$$

$$y_t = g(x_t, u_t) + v_t, \tag{2.12}$$

where $f(x_t, u_t)$ and $g(x_t, u_t)$ are known functions, w_t and v_t are uncorrelated Gaussian noises, and the signals y_t and u_t are known.

In this context, we have:

$$p(x_1) = \mathcal{N}\left(x_1; \mu_1, \Sigma_1\right), \tag{2.13}$$

$$p(x_t|y_{1:t}) \approx \mathcal{N}\left(x_t; \hat{x}_{t|t}, \Sigma_{t|t}\right), \tag{2.14}$$

$$p(x_{t+1}|y_{1:t}) \approx \mathcal{N}\left(x_{t+1}; \hat{x}_{t+1|t}, \Sigma_{t+1|t}\right), \tag{2.15}$$

where $p(x_1)$ represents the initial distribution of the state x_1, $p(x_t|y_{1:t})$ is the posterior distribution of the state x_t given all measurements up to time t, and $p(x_{t+1}|y_{1:t})$ is the predictive distribution of the state x_{t+1} given all measurements up to time t. The EKF equations reduce to:

$$K_t = \Sigma_{t|t-1} C_t^T (R + C_t \Sigma_{t|t-1} C_t^T)^{-1}, \tag{2.16}$$

$$\hat{x}_{t|t} = \hat{x}_{t|t-1} + K_t \left(y_t - g(\hat{x}_{t|t-1}, u_t) \right), \tag{2.17}$$

$$\Sigma_{t|t} = (I - K_t C_t) \Sigma_{t|t-1}, \tag{2.18}$$

$$\hat{x}_{t+1|t} = f(\hat{x}_{t|t}, u_t), \tag{2.19}$$

$$\Sigma_{t+1|t} = Q + A_t \Sigma_{t|t} A_t^T, \tag{2.20}$$

initialized with $\hat{x}_{1|0} = \mu_1$ and $\Sigma_{1|0} = \Sigma_1$.

In each iteration of the algorithm, the Jacobian matrices of the system are calculated based on the currently estimated state, resulting in time-varying matrices A_t and C_t. This local linearization is crucial for approximating the nonlinear behavior of the system to a linear model around the system's operating point. Thus, to implement the EKF algorithm described by equations (2.16)-(2.20), the following equalities must be utilized:

$$A_t = \left. \frac{\partial f_\Delta(x_t, u_t)}{\partial x_t} \right|_{x_t = \hat{x}_{t|t}},$$
$$C_t = \left. \frac{\partial g_\Delta(x_t, u_t)}{\partial x_t} \right|_{x_t = \hat{x}_{t|t-1}}.$$

2.1.3. Particle Filter

The Particle Filter (PF) is a nonlinear filtering algorithm based on the Monte Carlo method to approximate integrals involved in Bayesian estimation. It uses a set of weighted samples (particles) that represent the state distribution at each time step. By propagating these particles through the nonlinear system functions, state estimates can be obtained as a weighted sum of all particles [23]. The fundamental idea is to randomly select a set of weighted particles in the state space; according to the measurement results, the weights of the particles are continuously adjusted, and the state is recursively updated. The bootstrap version of this algorithm can be summarized in the following steps:

1. **Initialization:** Generate a set of particles following a known initial probability distri-

bution. Assign the same initial weight to each particle.

$$x_1^{(i)} \sim \mathcal{N}(\mu_1, \Sigma_1) \tag{2.21}$$

2. **Prediction:** Update each particle according to the system's transition model.

$$x_t^{(i)} \sim p(x_t \mid x_{t-1}^{(i)}) \tag{2.22}$$

3. **Update:** Calculate new weights based on the observed measurements and the system model.

$$w_t^{(i)} \propto p(y_t \mid x_t^{(i)}) \tag{2.23}$$

   These weights are then normalized.

4. **Resampling:** Select a new set of particles for replacement, taking into account their updated weights. Particles with higher weights have a higher probability of being chosen. Various resampling algorithms exist, such as Multinomial, Residual, Stratified, and Systematic resampling.

5. **State Estimation:** Calculate the state estimate using the particles selected after resampling.

$$\hat{x}_t = \sum_{i=1}^{M} w_t^{(i)} x_t^{(i)} \tag{2.24}$$

6. Move to the next time step and repeat steps 2 to 5.

The PF is more flexible than the EKF because it can handle systems with non-Gaussian noise. However, it may require a larger number of particles to obtain accurate estimations, which implies higher computational costs.

2.2. Model Predictive Control

Model Predictive Control (MPC) is an advanced control strategy that utilizes a mathematical model of the system and its current state to optimally determine future control inputs over a finite prediction horizon. The optimization process respects constraints that define allowable ranges for inputs, outputs, and system states [24].

MPC operates by solving an optimization problem at each sampling time. Based on the current state of the system, MPC predicts future behavior over a specified prediction horizon and computes the control actions that minimize a predefined cost function while ensuring compliance with system constraints. Only the first control action from the solution is applied, and the process is repeated at subsequent sampling times with updated state information. By incorporating future predictions and constraints, MPC effectively handles complex systems with multivariable interactions, time delays, and operational constraints.

MPC consists of four main components:

- **Mathematical model of the system:** Typically represented as a discrete-time state-space model to describe system dynamics. The model can be linear, nonlinear, or hybrid, depending on the system's characteristics.
- **Control horizon of N steps:** Specifies the number of future control actions calculated at each time step. It determines how far into the future the controller plans its actions.
- **Constraints on inputs, outputs, and states:** Define the permissible ranges for system variables, ensuring compliance with physical limits such as actuator saturation or safety bounds.
- **Cost function:** A quadratic cost function is commonly used to penalize deviations from the reference trajectory and excessive control effort. Alternative cost functions can be employed based on the application.

The effectiveness of MPC depends on the accuracy of the system model. An inaccurate model can lead to suboptimal or destabilizing control actions, whereas a well-calibrated model improves prediction accuracy and control performance. Real-time techniques like parameter identification and state estimation (e.g., Extended Kalman Filters) are often used to enhance model accuracy.

Another critical aspect is the optimization algorithm. Linear MPC typically uses quadratic programming (QP) solvers for efficient computation. Nonlinear MPC (NMPC), which handles nonlinearities, requires advanced algorithms like Sequential Quadratic Programming (SQP) or interior-point methods. While these methods offer flexibility, they are computationally more intensive.

MPC is widely applied in industries that require precise control of multivariable systems with time delays, such as chemical process control, energy management, and robotics. Its ability to handle time-varying constraints and objectives makes it ideal for dynamic environments.

2.2.1. Model Predictive Control for linear systems

The discrete-time linear model is described by the state-space equations:

$$x_{t+1} = Ax_t + Bu_t, \tag{2.25}$$

$$y_t = Cx_t + Du_t, \tag{2.26}$$

where $x_t \in \mathbb{R}^n$ is the system state, and x_0 is assumed to be known. $y_t \in \mathbb{R}$ is the output, and u_t is the control input, subject to the constraints:

$$u_t \in \mathcal{U}, \forall t \geq 0, \tag{2.27}$$

where $\mathcal{U} \subset \mathbb{R}$ defines the admissible input range.

The quadratic cost function V_N is defined as:

$$V_N(x_0, u_t) = x_N^T Q_N x_N + \sum_{t=0}^{N-1} \left(x_t^T Q x_t + u_t^T R u_t \right), \tag{2.28}$$

where Q and R are weight matrices for state and input costs, respectively, and Q_N is a terminal cost determined by the discrete-time algebraic Riccati equation (DARE). The optimal control problem is formulated as:

$$u^* = \arg\min_{u \in \mathcal{U}_N} V_N(x_0, u), \tag{2.29}$$

subject to:

$$x_{t+1} = Ax_t + Bu_t, \tag{2.30}$$

$$u_t \in \mathcal{U}, \forall t \in \{0, \dots, N-1\}, \tag{2.31}$$

$$x_N \in \mathcal{X}_f, \tag{2.32}$$

$$x_0 = \hat{x}_{t|t} \tag{2.33}$$

where $\mathcal{X}_f$ is the set of admissible terminal states. The feedback strategy involves solving the optimization problem at each sampling time and applying the first element of u^*.

In summary, Model Predictive Control offers a robust framework for managing constrained, multivariable systems. Its reliance on accurate models and real-time optimization has made it a cornerstone of advanced control strategies in modern engineering. The next section will explore Nonlinear Model Predictive Control (NMPC), which addresses the limitations of linear assumptions for systems with nonlinear dynamics.

2.2.2. Nonlinear Model Predictive Control (NMPC)

Nonlinear Model Predictive Control (NMPC) is an advanced control technique designed to manage systems with significant nonlinear behavior. While linear models are effective for systems with approximately linear dynamics, they often fail to capture the complexities of systems that exhibit strong nonlinear interactions between variables. In contrast, NMPC utilizes nonlinear mathematical models that better describe the intricate dynamics of these systems, enabling more precise control in scenarios where linear control methods would be insufficient.

A key challenge in NMPC is dealing with uncertainties, disturbances, and discrepancies between the model and the actual plant. The real system behavior often deviates from the predicted behavior due to factors such as unmodeled dynamics, sensor noise, and external disturbances. NMPC addresses this challenge by incorporating a feedback mechanism, where only open-loop manipulated inputs are applied until the next measurement is available. At each sampling period, the controller adjusts its predictions and recalculates the optimal inputs based on the latest measurements, allowing the system to dynamically respond to changing conditions. This iterative process ensures that the control inputs remain optimal as the system evolves.

The formulation of NMPC is based on a nonlinear system represented by the following state-space equations:

$$x_{t+1} = f(x_t, u_t) \tag{2.34}$$

$$y_t = g(x_t, u_t) \tag{2.35}$$

where $f(x_t, u_t)$ is a nonlinear function representing the system dynamics, and $g(x_t, u_t)$ is the nonlinear measurement function that models how the states are observed through available measurements.

In this thesis, NMPC is employed with a specific approach known as the delta formulation. This formulation, which introduces changes in the control input (δu) instead of directly using the control signal u, provides additional robustness in cases where actuator uncertainty or gain variations are present. The details of this formulation are discussed in the following section.

2.2.3. NMPC: Delta Formulation

The delta formulation (δu) arises naturally in systems where actuators may experience uncertainties, such as unknown or varying gains, or in systems prone to drift. Instead of calculating absolute control inputs, it is often more practical to compute the incremental changes (δu) in the control signals. This approach allows for better handling of actuator uncertainty and provides smoother control performance.

Based on [25], the NMPC scheme using the delta formulation modifies the control input as:

$$x_{t+1} = f(x_t, u_t) \tag{2.36}$$

$$u_t = u_{t-1} + \delta u_t \tag{2.37}$$

$$y_t = g(x_t, u_t) \tag{2.38}$$

Here, u_t is the control input at time t, and the change in the control input, δu_t, is treated as the decision variable in the optimization process. This formulation introduces an extra layer of robustness, as the controller adjusts for discrepancies in the system actuators while ensuring stable operation.

The NMPC optimization problem in the delta formulation is defined as:

$$J = \min_{\delta u_0, \ldots, \delta u_{N-1}} ||y_t - y_{\text{ref}}||_Q^2 + ||\delta u_t||_R^2 \tag{2.39}$$

$$\text{s.t.} \quad x_{t+1} = f(x_t, u_t), \quad t \geq 0 \tag{2.40}$$

$$y_t = g(x_t, u_t), \quad t \geq 0 \tag{2.41}$$

$$x_t \in \mathcal{X}, \quad u_t \in \mathcal{U}, \quad t = 0, ..., N-1 \tag{2.42}$$

$$x_N \in \mathcal{X}_f \tag{2.43}$$

$$x_0 = \hat{x}_{t|t} \tag{2.44}$$

$$u_t = u_{t-1} + \delta u_t, \quad t \geq 0 \tag{2.45}$$

$$u_{\min} \leq u_t \leq u_{\max} \tag{2.46}$$

$$\delta u_{\min} \leq \delta u_t \leq \delta u_{\max}, \tag{2.47}$$

where y_t is the system's output, y_{ref} is the reference signal to be tracked, $u_{\min}$ and $u_{\max}$ are the constraints on the inputs, $\delta u_{\min}$ and $\delta u_{\max}$ are the constraints on the input variations, and Q and R are weighting matrices that penalize deviations in the output and changes in the control input, respectively. The optimization is subject to the system dynamics and constraints on the state and control input.

The control input applied at time t is:

$$u_t = \delta u_t + u_{t-1} \tag{2.48}$$

This formulation ensures that the system eventually converges to a steady state where $\delta u_t \to 0$. At this point, the control input u_t and the system states x_t settle into a stable configuration, leading to accurate tracking of the reference signal y_{ref}. This property of the delta formulation is particularly beneficial in practical applications, where small adjustments in the control input can prevent excessive changes that could destabilize the system.

In practice, the delta formulation is widely used in industrial applications due to its ability to handle model mismatches and actuator non-linearities. It ensures smooth transitions in control actions and mitigates the impact of uncertainties in the system. As demonstrated in [26], NMPC with a delta formulation has proven to be effective in achieving precise tracking without the need for additional complexity in the control law design.

2.3. Parameter Identification

Parameter identification is a fundamental process in control systems, state estimation, and system modeling, particularly when dealing with nonlinear systems. The main objective is to estimate the values of key parameters that characterize the system's behavior based on experimental or observational data. Accurate identification of these parameters allows for a better understanding of the system's dynamics, which is essential for predicting responses to different inputs and designing robust control strategies.

In nonlinear systems, this task becomes significantly more challenging due to the complex and often intricate relationships between variables. Unlike linear systems, where the variables interact proportionally, nonlinear models involve interactions that may be influenced by phenomena such as saturation, hysteresis, and time delays, making traditional identification methods less effective. The presence of these nonlinearities demands more advanced techniques and computational tools to capture the true behavior of the system accurately.

Advances in computational power and algorithm development have greatly enhanced our ability to solve these complex problems. Techniques like gradient-based optimization, genetic algorithms, and machine learning approaches have been employed to refine parameter identification in nonlinear systems. These tools enable the automation of parameter tuning, which was once an arduous and time-consuming process, allowing researchers and engineers to identify parameters with greater accuracy and efficiency.

Parameter identification in nonlinear models not only helps in understanding the system's internal mechanisms but also serves as a critical foundation for designing effective control systems. Precise parameter estimation can lead to improved control performance, stability, and robustness, especially in dynamic systems where the parameters might change over time. This is particularly relevant in industries such as robotics, chemical processing, aerospace, and bioengineering, where the systems under control exhibit strong nonlinear behavior.

The methodology adopted in this thesis applies well-established optimization techniques to address the challenges of nonlinear parameter identification, particularly in the presence of noisy data, disturbances, and model inaccuracies. This approach offers a systematic and effective way to estimate parameters in complex systems, ultimately contributing to improved control design and overall system performance.

2.3.1. Identification Using Maximum Likelihood

One of the most widely used methods for parameter identification is Maximum Likelihood (ML) estimation. This method is particularly useful for nonlinear systems, as it provides a way to estimate parameters that maximize the likelihood of the observed data, given a particular model structure. The ML approach is grounded in statistical principles and takes into account the presence of measurement noise, disturbances, and other sources of error.

In the context of nonlinear systems, the input-output relationship is described by a nonlinear function $f(x_t; \theta)$, where θ represents the vector of unknown parameters to be identified. The system output is given by:

$$y_t = f(x_t; \theta) + w_t \tag{2.49}$$

where w_t represents the measurement noise, typically assumed to follow a Gaussian distribution with zero mean and variance σ^2, $N(0, \sigma^2)$. The aim of the identification process is to estimate the parameter vector θ such that the model output matches the observed data as closely as possible.

To accomplish this, the prediction error $\varepsilon_t(\theta)$, defined as the difference between the observed output y_t and the predicted output $\hat{y}_{t|t-1}(\theta)$, is minimized:

$$\varepsilon_t(\theta) = y_t - f(x_t;\theta) \tag{2.50}$$

Given the data sets $y_{1:N}$ and $x_{1:N}$, the goal is to estimate $\beta = [\theta^T \quad \sigma]$, which includes both the system parameters and the noise variance. The likelihood function is expressed as:

$$L_N(\beta) = p(y_{1:N} \mid x_{1:N}, \beta) \tag{2.51}$$

The Maximum Likelihood estimation process aims to maximize this likelihood function. In practice, it is often more convenient to minimize the log-likelihood function, which leads to the definition of the cost functional $V(\theta)$:

$$V(\theta) = \frac{1}{N}\sum_{t=1}^{N} \varepsilon_t(\theta)^2 \tag{2.52}$$

This results in an optimization problem where the estimated parameters $\hat{\theta}_{ML}$ are those that minimize the cost functional:

$$\hat{\theta}_{ML} = \arg\min_{\theta} V(\theta) \tag{2.53}$$

In addition, the variance of the noise w_t can be estimated as:

$$\hat{\sigma}_{ML} = \frac{1}{N}\sum_{t=1}^{N} \varepsilon_t(\hat{\theta}_{ML})^2 \tag{2.54}$$

This Maximum Likelihood approach provides a powerful method for parameter identification, especially in the presence of noise and disturbances. By minimizing the prediction error, the estimated parameters allow for an accurate description of the system's behavior, enabling more precise predictions and improved control design. This method will be applied in the context of this thesis to identify the parameters of the nonlinear system under study, ensuring that the model used for control is as representative of the real system as possible.

3. Problem Statement

The objective of this research is to design and implement a robust control strategy for a chemical process known as anaerobic digestion (AD), which is used to transform organic waste into biogas. This biogas, primarily composed of methane, is a renewable source of energy and plays a critical role in sustainable energy production. The anaerobic digestion process occurs in the absence of oxygen and is highly nonlinear, involving several interdependent biological and chemical reactions. These reactions break down organic materials such as agricultural residues, food waste, and sewage sludge into biogas, which can be harnessed as a form of green energy.

Anaerobic digestion is a slow process, with retention times ranging from 20 to 30 days, depending on the specific composition of the organic waste and the operating conditions of the plant. This makes real-time control and monitoring challenging since the delayed dynamics of the process require long periods to obtain reliable system measurements and assess performance. Additionally, AD systems are sensitive to variations in input composition, pH levels, temperature, and microbial activity, which adds to the complexity of maintaining optimal process conditions.

To address these challenges, researchers have developed the Anaerobic Digestion Model No. 1 (ADM1), which provides a detailed mathematical representation of the anaerobic digestion process. The ADM1 model is a comprehensive nonlinear model consisting of 36 states and 30 inputs, capturing the intricate biological and chemical interactions within the digester. These states represent various concentrations of substrates, intermediates, and microorganisms involved in the digestion process. The model also includes a large set of parameters, which are calibrated using experimental data obtained from specialized laboratories focused on process chemistry. The ADM1 model has been extensively validated in prior studies, showing minimal error when compared to real plant data, thereby demonstrating its accuracy as a reliable digital twin of the actual anaerobic digestion process.

Given its proven reliability, the ADM1 model is proposed to be used as a surrogate for the real plant in this research, serving as the platform for developing and testing advanced control strategies. By leveraging the ADM1 model, it becomes possible to simulate and predict the system's behavior under various operating conditions, allowing for the design of more effective control schemes that can optimize biogas production, minimize process instability, and reduce the risk of process failure. The model also provides a safe and efficient environment for testing control strategies without interfering with actual plant operations, reducing the time and cost associated with experimental trials in industrial settings.

The challenge lies in designing a control strategy that can manage the nonlinear and time-delayed nature of the process while maintaining stability and robustness against disturbances such as fluctuations in feedstock quality, temperature variations, and changes in microbial activity. To address this, advanced control techniques such as Nonlinear Model Predictive Control (NMPC) and state estimation methods like the Extended Kalman Filter (EKF) will be explored. These techniques will enable real-time adjustments to the process variables, ensuring that the anaerobic digester operates within optimal conditions, maximizing biogas yield and ensuring process stability.

Moreover, the control strategy must account for the economic and environmental factors associated with anaerobic digestion, including maximizing methane production, minimizing energy consumption, and reducing greenhouse gas emissions. The integration of control algorithms with process monitoring tools will help enhance the operational efficiency of AD plants, contributing to the overall sustainability of waste management and energy production systems.

In summary, the problem this research seeks to address is the development of a robust and efficient control framework for the anaerobic digestion process, utilizing the ADM1 model as a digital twin of the real system. This framework will aim to overcome the challenges of process nonlinearity, time delays, and sensitivity to disturbances, with the ultimate goal of improving the efficiency and reliability of biogas production in industrial anaerobic digestion plants.

3.1. Anaerobic Digestion: ADM1 Simulator

Anaerobic digestion is a microbiological process that produces biogas, primarily composed of methane (CH_4) and carbon dioxide (CO_2), along with stabilized solid residues. This process occurs within specialized reactors, where a diverse community of microorganisms breaks down organic materials through several stages: hydrolysis, acidogenesis, acetogenesis, and methanogenesis [27, 28]. Each stage is governed by specific microbial populations with distinct environmental and nutrient requirements. The primary objective of anaerobic digestion is to convert complex organic compounds such as carbohydrates, proteins, and lipids into simpler molecules, which are then transformed into biogas.

One of the most widely accepted and extensively used mathematical frameworks to simulate and analyze this process is the Anaerobic Digestion Model No. 1 (ADM1). Developed by the International Water Association (IWA), ADM1 provides a standardized methodology for simulating anaerobic digestion in diverse applications, including wastewater treatment, agricultural waste management, and renewable energy production. This model has been fundamental in improving the understanding of the biochemical processes and interactions underlying anaerobic digestion.

ADM1 describes the anaerobic digestion process using a comprehensive system of nonlinear differential equations. These equations capture the dynamics of various substrates—such as sugars, amino acids, long-chain fatty acids, and volatile fatty acids (VFAs)—as they are transformed by different microbial groups. The model also accounts for the growth and decay of microbial populations in each stage, the production of intermediate metabolites and biogas (methane and carbon dioxide), and key operational factors such as pH, temperature, alkalinity, and the inhibitory effects of compounds like ammonia and sulfides, all of which significantly influence microbial activity and biogas production.

Due to its detailed representation, ADM1 is a powerful tool for researchers and plant operators. It allows prediction of anaerobic digester performance under varying feedstock compositions, operational conditions, and environmental factors. These predictive capabilities are essential for optimizing biogas production, improving process stability, and maximizing resource recovery from organic waste. Furthermore, ADM1 provides valuable insights into how process parameters such as organic loading rate (OLR), hydraulic retention time (HRT), and digester temperature can be adjusted to enhance efficiency.

Despite its accuracy and detail, the complexity of ADM1 poses challenges for real-time applications. The model comprises 36 state variables, 30 input parameters, and numerous rate equations, resulting in significant computational demand. Solving these equations in real time requires considerable resources, making ADM1 impractical for direct use in controller or estimator design for anaerobic digestion systems.

To overcome these limitations, ADM1 is often used as a virtual plant to generate experimental data under controlled conditions. These data can then calibrate and validate simplified models better suited for real-time control. In this research, a reduced model called Anaerobic Model No. 2 (AM2) is used. AM2 retains the essential dynamics of anaerobic digestion while significantly reducing the number of state variables and computational complexity, making it feasible for developing and implementing control strategies.

By leveraging ADM1 for detailed simulations and AM2 for control design, this approach combines the predictive power of ADM1 with the simplicity and efficiency of AM2. The AM2 model is crucial for designing advanced controllers and estimators, such as Nonlinear Model Predictive Control (NMPC) and the Extended Kalman Filter (EKF), to optimize anaerobic digestion. This strategy enables effective regulation of key process variables—such as pH, temperature, and organic loading—enhancing biogas production and improving overall process stability and sustainability.

3.2. AM2 Model

The AM2 dynamic model is a reduced mathematical model that describes the anaerobic digestion process of easily biodegradable waste [29, 30]. Although it has initially been calibrated for simulating the anaerobic digestion (AD) of winery distillery vinasses, the set of kinetic and stoichiometric parameters of the model could be adjusted for simulating any other organic waste, including co-digestion systems.

By applying control signals u_t, this model allows us to predict the process outputs y_t and the states x_t.

Based on the model described in [31], the AM2 model assumes that the process can be reduced to two main stages: acidogenesis, where the substrate S_1 is degraded by acidogenesis (X_1) and transformed into volatile fatty acids (S_2) and CO_2; methanogenesis, where the volatile fatty acids (VFA) are degraded into CH_4 and CO_2 by methanogenic archaea (X_2). This system can be represented by a continuous-time nonlinear state-space system, where the states are:

microbial degraders X_1 and X_2, organic substrates S_1 and S_2, alkalinity (Z), and inorganic carbon (C). These states are described by the following equations:

$$\dot{X}_1 = \mu_1 X_1 - \alpha D X_1 \tag{3.55}$$

$$\dot{X}_2 = \mu_2 X_2 - \alpha D X_2 \tag{3.56}$$

$$\dot{S}_1 = D(S_{1\text{in}} - S_1) - k_1 \mu_1 X_1 \tag{3.57}$$

$$\dot{S}_2 = D(S_{2\text{in}} - S_2) + k_2 \mu_1 X_1 - k_3 \mu_2 X_2 \tag{3.58}$$

$$\dot{Z} = D(Z_{\text{in}} - Z) \tag{3.59}$$

$$\dot{C} = D(C_{\text{in}} - C) - q_{\text{C}} + k_4 \mu_1 X_1 + k_5 \mu_2 X_2 \tag{3.60}$$

where

$$\varphi = C + S_2 - Z + k_{\text{H}} P_{\text{T}} + \frac{k_6}{k_{\text{La}}} \mu_2 X_2 \tag{3.61}$$

$$q_M = k_6 \mu_2 X_2 \tag{3.62}$$

$$pH = -\log_{10}\left(k_{\text{b}} \frac{C - Z + S_2}{Z - S_2}\right) \tag{3.63}$$

$$\mu_1 = \frac{\mu_1^{\max} S_1}{k_{\text{S1}} + S_1} \tag{3.64}$$

$$\mu_2 = \frac{\mu_2^{\max} S_2}{k_{\text{S2}} + S_2 + (S_2^2 / k_{\text{I2}})} \tag{3.65}$$

are nonlinear functions; C and C_{in} are the total inorganic carbon concentration [mmol/L]; D is the dilution rate [d^{-1}]; k_1 is the substrate degradation yield; k_2, yield of volatile fatty acid (VFA) production [mmol/g]; k_3, yield of VFA consumption [mmol/g]; k_4 and k_5, yield of CO_2 production [mmol/g]; k_6, yield of CH_4 production [mmol/g]; k_{b}, equilibrium constant [mol/L]; k_{H}, Henry's constant [mmol/L/atm]; k_{La}, liquid-gas transfer constant [d^{-1}]; k_{I2}, inhibition constant [mmol/L]; k_{S1}, half-saturation constant [g/L]; k_{S2}, half-saturation constant [mmol/L]; P_{C}, CO_2 partial pressure [atm]; P_{T}, total pressure [atm]; q_C, carbon dioxide flow rate [mmol/L/d]; q_{M}, methane flow rate [mmol/L/d]; S_1 and S_{1in}, organic substrate concentration [gCOD/L]; S_2 and S_{2in}, VFA concentration [mmol/L]; X_1, concentration of acidogens [g/L]; X_2, concentration of methanogens [g/L]; Z and Z_{in}, total alkalinity [mmol/L]; α is the fraction of bacteria in the liquid phase; μ_1, specific growth rate of acidogens [d^{-1}]; $\mu_1{}^{\max}$, maximum growth rate of acidogens [d^{-1}]; μ_2, specific growth rate of methanogens [d^{-1}]; $\mu_2{}^{\max}$, maximum growth rate of methanogens [d^{-1}].

Table 3.1 shows the values of the model parameters.

Parameter	**Value**	***Initial Condition***	**Value**
k_1	42.14	C_0	65
k_2	116.5	$C_{in,0}$	60
k_3	268	D_0	0.34
k_4	50.6	$S_{1,0}$	1.8
k_5	343.6	$S_{1in,0}$	9.5
k_6	453	$S_{2,0}$	3.0
k_{b}	$6.5 \cdot 10^{-7}$	$S_{2in,0}$	93.6
k_{H}	16	$X_{1,0}$	0.8
k_{La}	19.8	$X_{2,0}$	0.8
k_{I2}	256	Z_0	60
k_{S1}	7.1	$Z_{in,0}$	62.5
k_{S2}	9.28	α	0.5
$\mu_1{}^{\max}$	1.2	P_{T}	1
$\mu_2{}^{\max}$	0.74		

Table 3.1: Model Parameters

3.3. Previous Results

In the paper [31], a control algorithm using Nonlinear Model Predictive Control (NMPC) for the anaerobic digestion process (ADM1) was developed, employing the simplified AM2 model as the base for the controller. It was assumed that there was full access to the measurements of the ADM1 model, eliminating the need to estimate states to obtain complete system information. Additionally, measurement noise was not considered in the initial setup. The NMPC was configured to use a prediction and control horizon of 4 system sampling points, which corresponds to 0.1 days.

In the first scenario presented in the paper, as illustrated in Figures 3.1 and 3.2, Nonlinear Model Predictive Control (NMPC) was implemented using the AM2 model as the plant. This implementation validated the developed controller's ability to accurately follow the reference trajectory. The results indicated a strong tracking performance, which is crucial for maintaining the desired operational conditions in the anaerobic digestion process. Additionally, the simulations demonstrated the controller's robustness against disturbances, ensuring that the system could adapt to variations in input and maintain stability throughout the operation. This highlights the effectiveness of NMPC in optimizing the performance of complex nonlinear systems like anaerobic digesters.

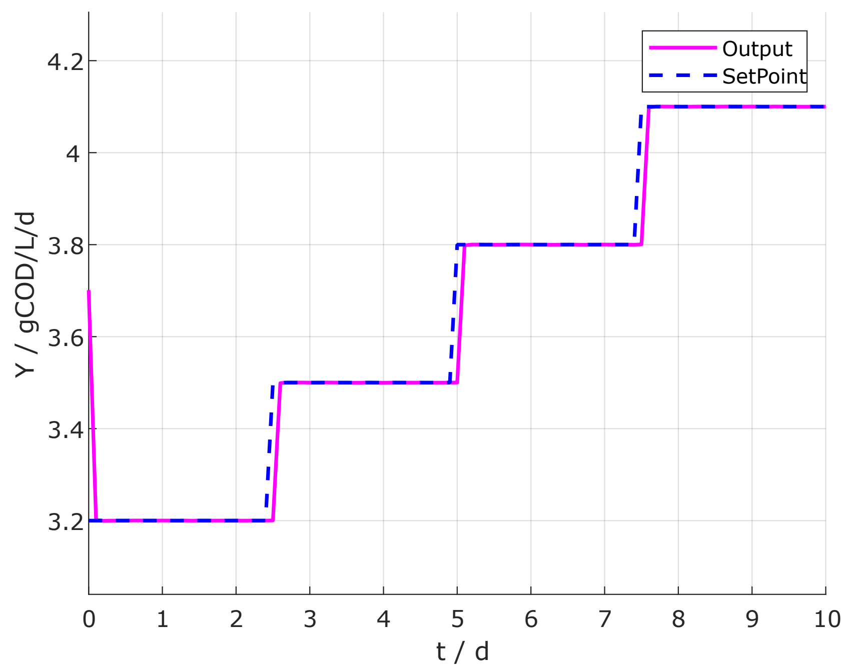

Figure 3.1: NMPC Output Plot Using AM2-AM2

In the second scenario of interest, an attempt was made to control the ADM1 process using NMPC with the AM2 model. Figures 3.3 and 3.4 show that the implemented algorithm managed to control the system and stabilize the process, albeit at a value different from the desired one, indicating the presence of a bias between the ADM1 and AM2 models. Despite

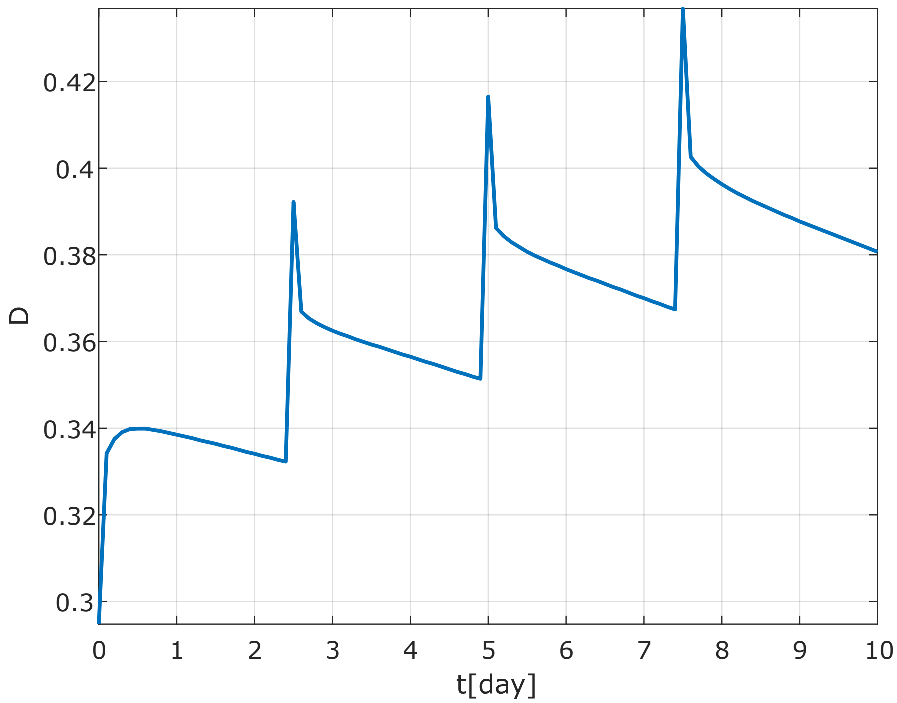

Figure 3.2: NMPC Input Plot Using AM2-AM2

this bias, a maximum error of 18% was achieved, which occurred in the last desired reference signal. This result was considered acceptable for controlling the anaerobic digestion process for lower reference levels.

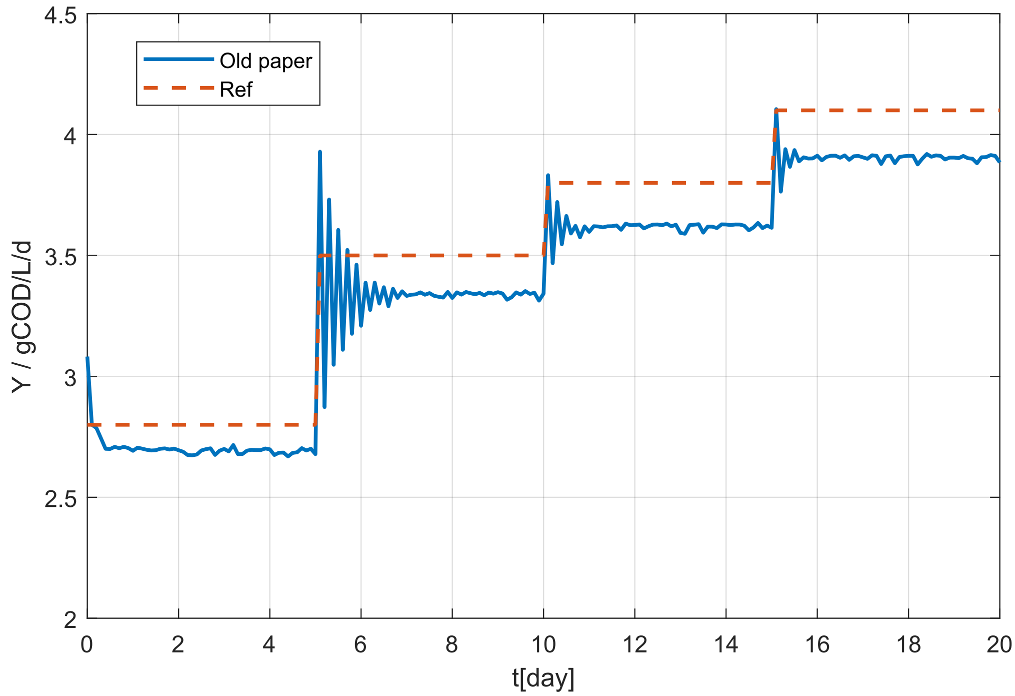

Figure 3.3: NMPC Output Plot Using AM2-ADM1

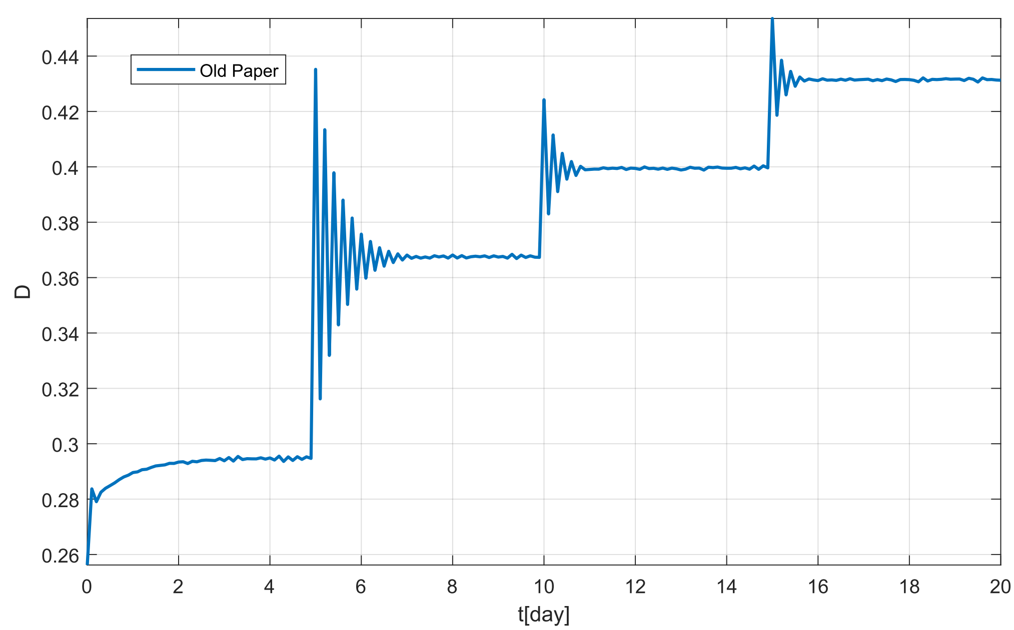

Figure 3.4: NMPC Input Plot Using AM2-ADM1

4. Problem Resolution

In this section, various techniques will be detailed to efficiently solve the control problem of the anaerobic digestion process. It is assumed that the tools used are well-known, as they were detailed in Chapter 2 on Concepts.

The AM2 process can be described as a nonlinear continuous-time state-space system, where the state variables represent microbial populations (X_1, X_2), organic substrates (S_1, S_2), alkalinity (Z), and inorganic carbon (C). Using vector notation, the model is expressed as follows:

$$\dot{\mathbf{x}} = f_c(\mathbf{x}, u), \tag{4.66}$$

$$y = g(\mathbf{x}), \tag{4.67}$$

where

$$\mathbf{x} = \begin{bmatrix} X_1 \\ X_2 \\ S_1 \\ S_2 \\ Z \\ C \end{bmatrix}, \quad f_c(\mathbf{x}, u) = \begin{bmatrix} \mu_1(S_1)X_1 - \alpha D X_1 \\ \mu_2(S_2)X_2 - \alpha D X_2 \\ D(S_{1in} - S_1) - k_1\mu_1(S_1)X_1 \\ D(S_{2in} - S_2) + k_2\mu_1(S_1)X_1 - k_3\mu_2(S_2)X_2 \\ D(Z_{in} - Z) \\ D(C_{in} - C) - q_C + k_4\mu_1(S_1)X_1 + k_5\mu_2(S_2)X_2 \end{bmatrix}, \quad g(\mathbf{x}) = k_6\mu_2(S_2)X_2. \tag{4.68}$$

where $f_c(\mathbf{x}, u)$ defines the nonlinear continuous-time dynamics of the system, and $g(\mathbf{x})$ represents the nonlinear output function that models the measurable output of the process.

4.1. Discretization of the Model

To implement the proposed control strategy on a digital platform, the continuous-time model must be discretized. The Euler method is selected for this purpose due to its simplicity and suitability for systems with slow dynamics. This method uses a discrete time step Δ, which defines the interval between successive samples. The discrete-time model is then given by:

$$x_{t+1} = x_t + \Delta f_c(x_t, u_t) = f(x_t, u_t), \tag{4.69}$$

$$y_t = g(x_t), \tag{4.70}$$

where x_t and x_{t+1} are the state vectors at times t and $t+1$, respectively; u_t is the control input at time t; and y_t is the output vector. The state vector x_t is defined as:

$$x_t = \begin{bmatrix} X_{1,t} \\ X_{2,t} \\ S_{1,t} \\ S_{2,t} \\ Z_t \\ C_t \end{bmatrix}. \tag{4.71}$$

In this formulation, $f(x_t, u_t)$ represents the discrete-time nonlinear dynamics derived from Euler integration of the continuous system described by $f_c(x_t, u_t)$, while $g(x_t)$ retains the same measurement function as in the continuous-time case.

Regarding the choice of the sampling time Δ, it is important to consider that anaerobic digestion is a slow biochemical process. In practical applications, it is common to sample the system once per day or even just a few times per week. For this study, a sampling interval of 0.1 days was selected. This choice offers a good compromise between adequately capturing the system's dynamics and avoiding excessive computational burden or the amplification of measurement noise due to overly frequent sampling.

4.2. State Estimation Implementation

The system considered within the AM2 framework for state estimation corresponds to a nonlinear discrete-time model of the form:

$$\begin{aligned} x_{t+1} &= f(x_t, u_t) + w_t, \\ y_t &= g(x_t, u_t) + v_t, \end{aligned} \tag{4.72}$$

where f and g represent the discretized versions of equations (4.69) and (4.70), respectively. The terms w_t and v_t denote white Gaussian noise processes, uncorrelated with x_t, with zero mean and known covariance matrices. The state vector is defined as:

$$x_t = \begin{bmatrix} x_t^{(1)} \\ x_t^{(2)} \\ x_t^{(3)} \\ x_t^{(4)} \\ x_t^{(5)} \\ x_t^{(6)} \end{bmatrix} = \begin{bmatrix} X_{1,t} \\ X_{2,t} \\ S_{1,t} \\ S_{2,t} \\ Z_t \\ C_t \end{bmatrix} \tag{4.73}$$

4.2.1. Implementation of Filtering Algorithms

State estimation was previously studied in [32], which forms part of the research developed in this thesis. That work focused on the observability analysis of the AM2 system and assessed the performance of two estimation algorithms designed for nonlinear systems: the Extended Kalman Filter (EKF) and the Particle Filter (PF).

An observability study of the AM2 model revealed limitations in estimating the states $x_t^{(5)}$ and $x_t^{(6)}$. Similar issues were also reported in [13], where unknown inputs were treated as additional states to be estimated. In contrast, this thesis assumes that the inputs are known, as they are generated by the NMPC controller. This assumption simplifies the estimation task by focusing the filters solely on the internal system states. For linear systems, as noted in [33], convergence of the Kalman filter is guaranteed if the system is at least detectable—an assumption extended here to the nonlinear case.

To evaluate the filters performance, a discrete-time simulation was performed where a constant input u_t, equal to the initial condition, was applied. Gaussian white noise with variances

$Q = 0.001$ (process noise) and $R = 0.01$ (measurement noise) was added to emulate real-world disturbances. Both the EKF and PF (with 1000 particles) were implemented to estimate the system states. A Monte Carlo simulation of 100 runs was conducted, each with the same initial conditions but different noise realizations.

As shown in Figure 4.5, the average trajectories estimated by both filters closely match the true state trajectories generated by the AM2 model, demonstrating the general effectiveness of both algorithms. However, when analyzing individual runs, the PF exhibits significant dispersion, whereas the EKF provides more stable and consistent estimates across simulations. This is further illustrated in Figure 4.6, where the PF shows wider interquartile ranges in the boxplots, indicating greater variability in performance, while the EKF results are more tightly clustered around the mean.

An exception was noted in the estimation of state $x_t^{(5)}$. Both filters exhibited a transient bias during the initial phase, which gradually diminishes as the filters converge. For the EKF, this bias is consistent across simulations, while the PF showed a smaller but more variable deviation in each run. This should be taken into account in applications requiring precise estimation of this particular state.

Table 4.2 summarizes the average computation times, showing that the EKF is at least ten times faster than the PF.

Table 4.2: Average Estimation Time (seconds)

Algorithm	Execution Time
EKF	0.0040 ± 0.0038
PF	0.0654 ± 0.0113

An additional simulation was performed in which the noise variances were slightly increased and the initial conditions were varied for each realization. The results, shown in Figure 4.7, indicate that both filters exhibit similar behavior, effectively ruling out the anomaly observed in the previous scenario as a general issue. However, the difficulty in accurately estimating state $x_t^{(5)}$ persists, suggesting a possible observability issue specific to this variable. As a result, it is recommended to exclude this state from future implementations or to investigate alternative estimation strategies for improved performance.

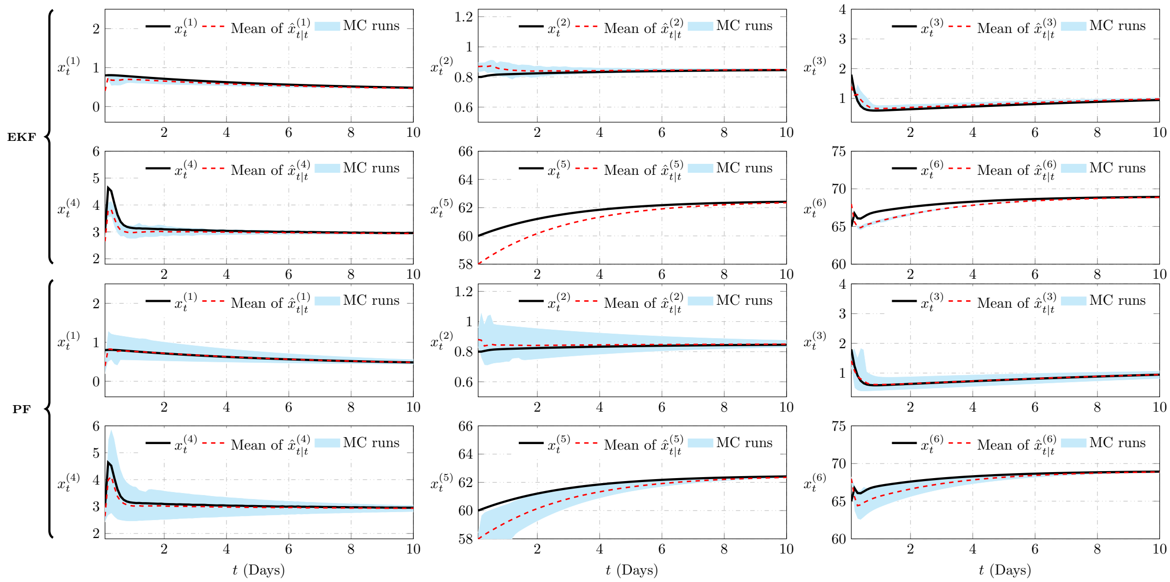

Figure 4.5: State estimations using EKF and PF (100 realizations).

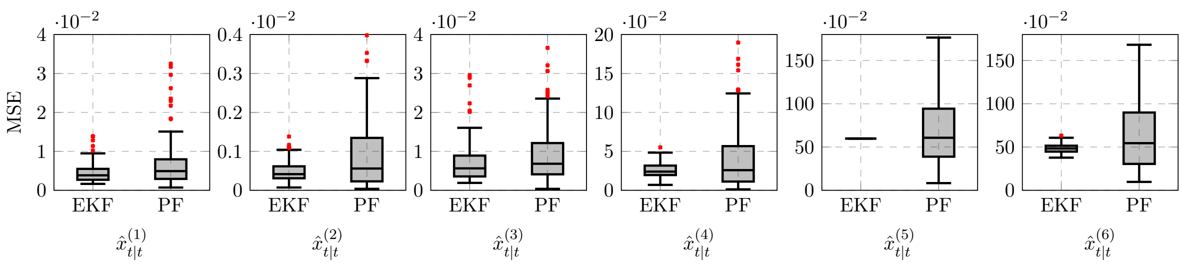

Figure 4.6: Boxplot of state estimation errors using EKF and PF (100 realizations).

This study assessed state estimation in an anaerobic digestion model using the Extended Kalman Filter (EKF) and the Particle Filter (PF). After discretizing the model, both algorithms were implemented and compared. The EKF demonstrated superior accuracy and was significantly faster than the PF with 100 particles. Monte Carlo analysis revealed that PF estimates were more variable, while EKF remained more consistent. Based on these results, the EKF was selected as the state estimation filter for this work due to its balance of accuracy and computational efficiency.

4.2.2. Modification to AM2 Model

Based on the previous analysis, a modified version of the AM2 system was selected. This corresponds to a Single Input Single Output (SISO) configuration with four states. The input

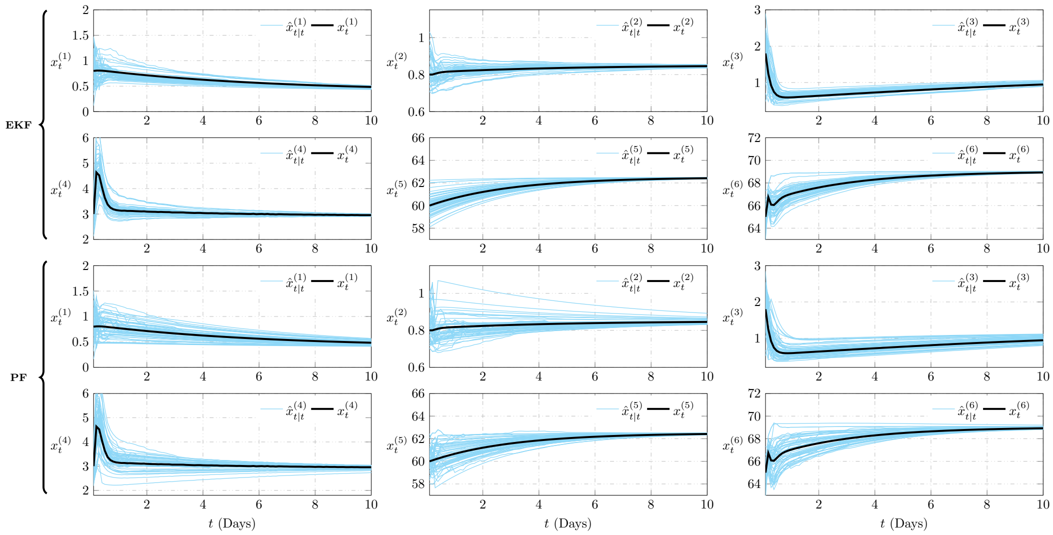

Figure 4.7: State estimates obtained using EKF and PF. 100 realizations with different initial conditions.

signal is defined as $u = D$, representing the dilution rate, while the output signal is $y = q_M$, denoting the production rate of the desired metabolites. The system states are defined as follows:

$$\dot{X}_1 = \mu_1 X_1 - \alpha D X_1 \tag{4.74}$$

$$\dot{X}_2 = \mu_2 X_2 - \alpha D X_2 \tag{4.75}$$

$$\dot{S}_1 = D(\bar{S}_{1\text{in}} - S_1) - k_1 \mu_1 X_1 \tag{4.76}$$

$$\dot{S}_2 = D(\bar{S}_{2\text{in}} - S_2) + k_2 \mu_1 X_1 - k_3 \mu_2 X_2 \tag{4.77}$$

where $\bar{S}_{1\text{in}}$ and $\bar{S}_{2\text{in}}$ are constants that represent the initial concentrations of the substrates in the system. The new corresponding state vector is given by:

$$x_t = \begin{bmatrix} x_t^{(1)} \\ x_t^{(2)} \\ x_t^{(3)} \\ x_t^{(4)} \end{bmatrix} = \begin{bmatrix} X_{1,t} \\ X_{2,t} \\ S_{1,t} \\ S_{2,t} \end{bmatrix} \tag{4.78}$$

This modification to the AM2 system was implemented for the following reasons:

- **Discarding the states Z and C:** These states do not significantly influence the system dynamics in terms of output estimation. They are primarily utilized for calculating the system's pH, which is a factor that will be considered as a constraint for the controller in future analyses. Furthermore, previous studies have indicated that these states are not observable, thus justifying their exclusion from the model.

- **Changing from MISO to SISO:** The complexity associated with multiple input signals was reduced by discarding the states associated with Z_{in} and C_{in}. Instead, we focused on integrating the two main substrate inputs, $S_{1\text{in}}$ and $S_{2\text{in}}$, into the controller design. This adjustment allows for a more straightforward implementation of control strategies that are inherently more effective in SISO systems, particularly considering that the previously included input signals had restrictions limiting their variability over time.

4.2.3. Implementation of EKF in AM2 and ADM1 Models

As discussed in the previous sections, the Extended Kalman Filter (EKF) was selected for state estimation. This section presents the results obtained by applying the EKF to both the AM2 and ADM1 models. Simulations are performed in two scenarios: one using data generated by the AM2 model, and another using data from the more complex ADM1 model.

Figure 4.8 shows the EKF state estimates obtained with data simulated from the AM2 model. The red lines represent the true state trajectories, while the green lines depict the EKF estimates along with the 99% confidence intervals. The sampling time was set to 0.1 days, reflecting the slow dynamics of the anaerobic digestion process. The EKF accurately tracks the states, with minimal bias and well-behaved confidence intervals, demonstrating its suitability for this model.

In contrast, Figure 4.9 presents the EKF estimates when applied to data generated by the more complex ADM1 model. While the estimates initially follow the true states, their accuracy degrades over time, particularly for state X_4, where significant divergence occurs. This behavior is attributed to the structural mismatch between models: ADM1 has 36 states, whereas AM2

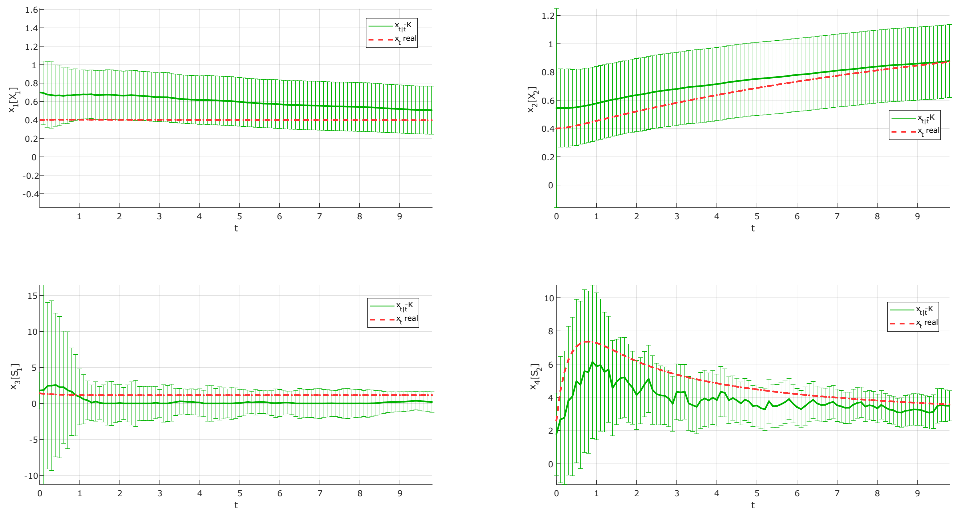

Figure 4.8: State estimation results for the AM2 model using EKF.

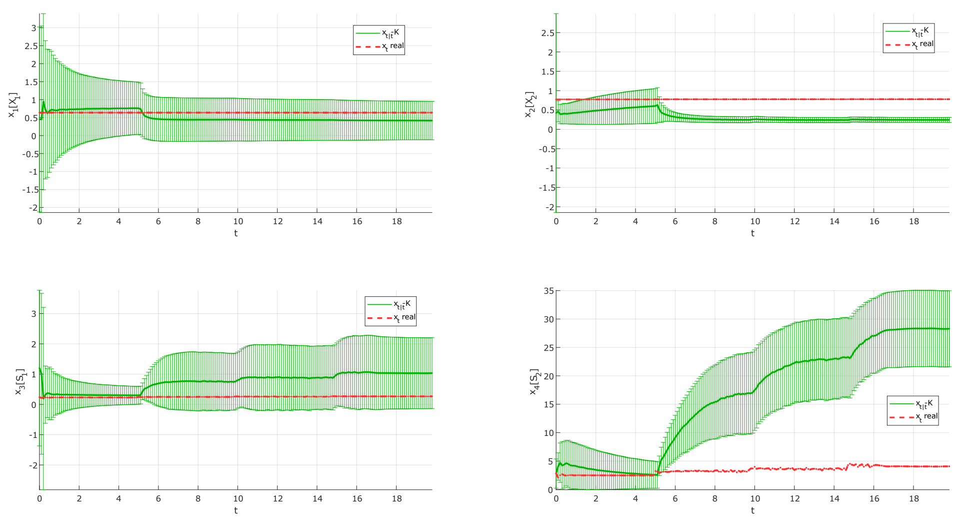

Figure 4.9: State estimation results for ADM1 data using EKF with the AM2 model.

is a simplified 4-state model. As the operating conditions vary, the simplified model fails to capture the full dynamics of ADM1, resulting in increasing estimation errors.

Despite these limitations, the EKF implementation is validated as a reliable estimator, though some bias is observed in specific states. To address this, incorporating an integral action in the controller is proposed to correct steady-state offsets and improve overall control performance.

In summary, the EKF is an effective state estimator for nonlinear models like AM2. Future work may focus on enhancements such as adaptive filtering techniques to increase robustness against model uncertainties and external disturbances.

4.3. NMPC Control Implementation

To implement Nonlinear Model Predictive Control (NMPC) in plants, it is essential to note that typically only the system measurements y_t are available. Consequently, the Extended Kalman Filter (EKF) developed in the previous section has been integrated into this control strategy to provide state estimates $\hat{x}_t$. When using the EKF, the model f is employed to predict the system's behavior. Specifically, the following model is utilized:

$$x_{t+1} = f(x_t, u_t), \tag{4.79}$$

$$y_t = g(x_t, u_t), \tag{4.80}$$

The NMPC framework, as detailed in Chapter 2, builds upon a previously established algorithm, incorporating modifications to meet the requirements of the simplified discrete AM2 model, defined earlier in this chapter as f.

Once the state estimates are obtained, they are used to define the NMPC optimization problem. The optimization problem is formulated as follows, with the objective of minimizing a cost function that penalizes deviations from the desired system result and excessive control effort:

$$J = \min_{\delta u_0, \ldots, \delta u_{N-1}} ||y_t - y_{\text{ref}}||_Q^2 + ||\delta u_t||_R^2 \tag{4.81}$$

$$\text{s.t.} \quad x_{t+1} = f(x_t, u_t), \quad t \geq 0 \tag{4.82}$$

$$y_t = g(x_t, u_t), \quad t \geq 0 \tag{4.83}$$

$$x_t \in \mathcal{X}, \quad u_t \in \mathcal{U}, \quad t = 0, \ldots, N-1 \tag{4.84}$$

$$x_N \in \mathcal{X}_f \tag{4.85}$$

$$u_t = u_{t-1} + \delta u_t, \quad t \geq 0 \tag{4.86}$$

$$x_0 = \hat{x}_{t|t} \tag{4.87}$$

$$u_{\min} \leq u_t \leq u_{\max} \tag{4.88}$$

$$\delta u_{\min} \leq \delta u_t \leq \delta u_{\max}, \tag{4.89}$$

Finally, the first optimal control action of δu_t, is applied to the system, updating the control input:

$$u_t = \delta u_t + u_{t-1}. \tag{4.90}$$

In this study, a simulation was conducted aiming to control the anaerobic digestion plant modeled by ADM1 over a period of 20 days, employing a sampling time of 0.1 days. Throughout this duration, four distinct set points were established, with changes occurring every five days. The results of the simulation are depicted in Figures 4.10, 4.11 and 4.12, illustrating the output, estimation and input profiles, respectively.

The results indicate that the application of the NMPC controller, in conjunction with the EKF, effectively stabilizes the system. However, a noticeable bias relative to the desired set points remains. This error tends to increase in proportion to the set point value, culminating in a maximum deviation of 15.4% in terms of reference tracking. Furthermore, as shown in Figure 4.11, the estimates generated by the EKF diverge from the actual system values for each set point, suggesting that the AM2 model is not sufficiently calibrated to replicate the dynamics of the ADM1 model accurately.

Despite the considerable discrepancies in the state estimates, the reference tracking performance in this scenario surpasses that of the previous section, where actual state values were directly available. This improvement is attributed to the EKF's corrective capabilities in addressing measurement errors to derive state estimates. Nevertheless, this correction mechanism alone is insufficient to yield satisfactory results within the implemented NMPC control system.

An important observation from the simulation results is that at lower set points, the AM2 process tends to mimic the ADM1 system more closely. Conversely, as the set points increase, the AM2 model increasingly diverges from the real system, leading to significantly larger biases for each utilized set point. This behavior may arise from specific internal dynamics within the ADM1 process that the AM2 model fails to capture accurately.

To address these discrepancies and enhance the overall performance of the control system, it is proposed to implement certain improvements. These modifications will focus on refining the

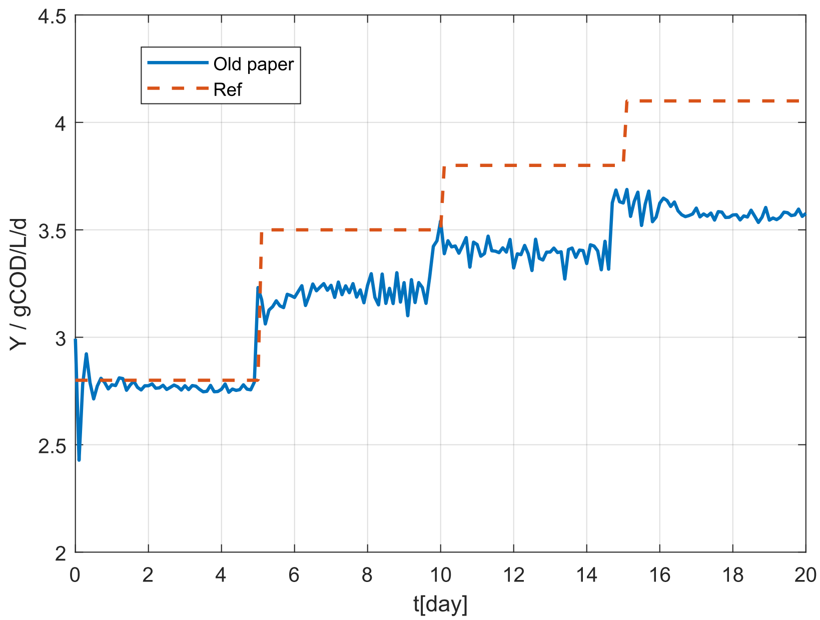

Figure 4.10: NMPC Output Graph using AM2 and EKF

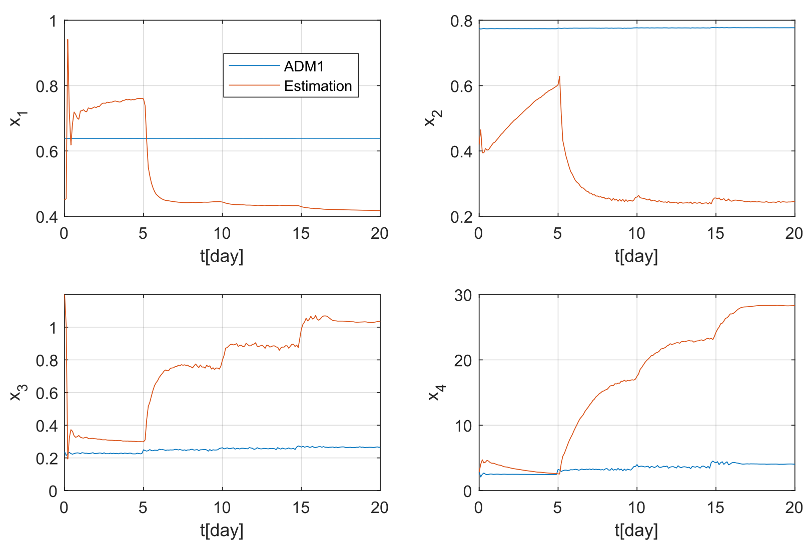

Figure 4.11: NMPC Estimation Graph using AM2 and EKF

NMPC approach and integrating adaptive control strategies that can dynamically adjust the controller parameters based on real-time feedback from the system. Such enhancements aim to bridge the gap between the AM2 and ADM1 models, ultimately leading to more accurate and robust control of the anaerobic digestion process. The details of these proposed improvements

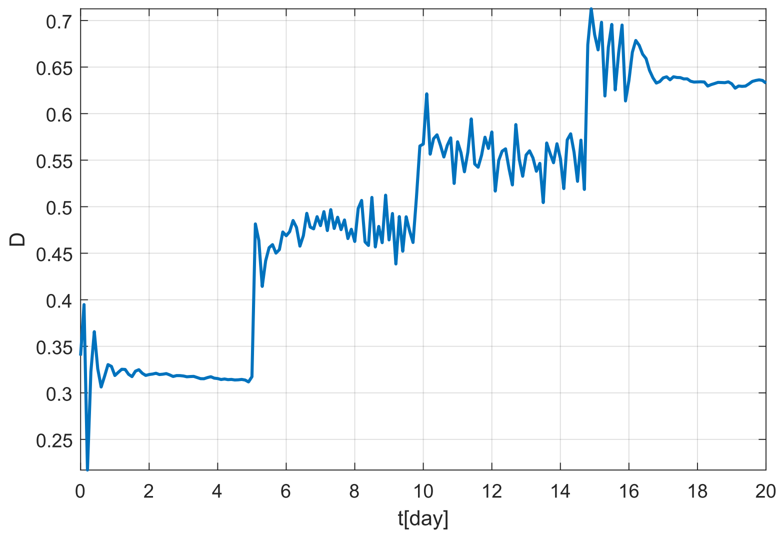

Figure 4.12: NMPC Input Graph using AM2 and EKF

will be elaborated in the subsequent section.

4.4. Improvements to Control Implementation

This section introduces two key tools aimed at enhancing the performance of the NMPC controller for the ADM1 process, with the primary objective of minimizing reference tracking errors across various desired output values.

4.4.1. Parameter Identification Implementation

A significant discrepancy was identified between the AM2 model and the ADM1 model, particularly in the output equation related to methane flow (CH_4). To address this, we propose adjusting parameters within the AM2 output equation to improve its alignment with the ADM1 model through a parameter identification process.

The output equation of the AM2 model is expressed as follows:

$$y_{\mathrm{AM2}} = k_6 X_2 \mu_2(S_2), \quad \mu_2(S_2) = \frac{\mu_2^{\max} S_2}{k_{\mathrm{S2}} + S_2 + \left(\frac{S_2^2}{k_{\mathrm{I2}}}\right)}. \tag{4.91}$$

This equation consists of four parameters that require adjustment: k_6, $\mu_2^{\max}$, k_{S2}, and k_{I2}.

To carry out this adjustment, we employed a nonlinear fitting method based on Maximum Likelihood estimation, with the aim of minimizing the mean squared error between experimental data obtained from the ADM1 model and the nonlinear output defined in (4.91). The results of this parameter fitting are summarized in Table 4.3.

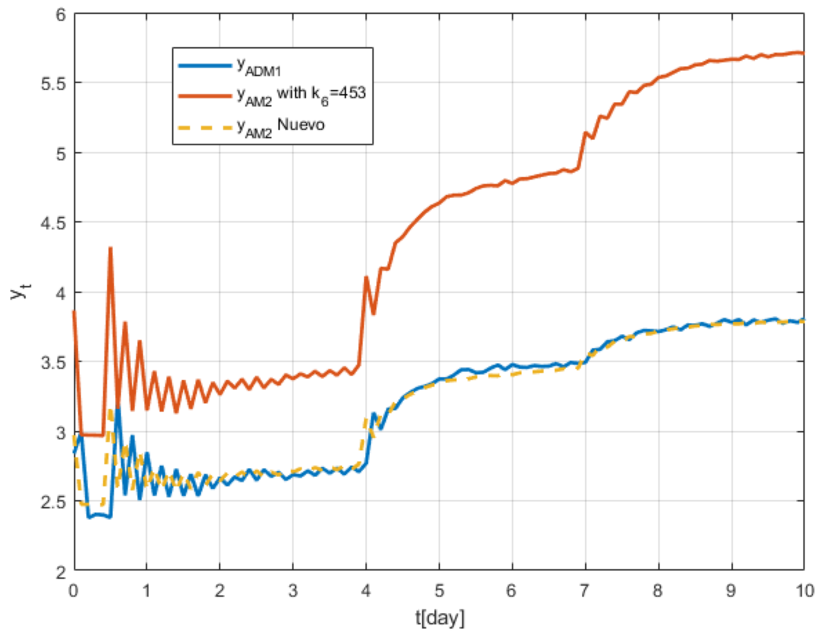

Figure 4.13: Adjusted AM2 Model Output - Latest Version

Using these optimized parameter values, the AM2 model was re-simulated. Figure 4.13 illustrates a comparison of output signals: the blue trace represents actual plant data obtained from the ADM1 model, the orange trace indicates the output from the AM2 model without parameter adjustments, and the yellow trace depicts the output from the AM2 model using the adjusted parameters. The graph demonstrates a significant improvement in the AM2 model's performance, closely approximating the behavior of the ADM1 model.

Parameter	Old Value	New Value
k_6	453	457.73
$\mu_2^{\max}$	0.74	0.2688
k_{S2}	9.28	2.9524
k_{I2}	256	383.977

Table 4.3: Parameters obtained using Maximum Likelihood estimation

4.4.2. Integral Action for EKF-NMPC controller

Given that there will inevitably be discrepancies between the estimated states of the reduced model and the actual values particularly at higher reference values we propose the incorporation of integral action into the control system. This adjustment is intended to eliminate steady state error.

To achieve this, we introduce an additional state, d_t, which represents a constant disturbance reflecting the difference between the AM2 and ADM1 models, thereby compensating for the error between them. The modified state-space representation is given by:

$$x_{t+1} = f(x_t, u_t + d_t) + w_t \tag{4.92}$$

$$d_{t+1} = d_t + s_t, \tag{4.93}$$

$$y_t = g(x_t, u_t) + v_t, \tag{4.94}$$

This system can be expressed in matrix form, with the definition of an extended state vector:

$$\mathcal{X}_{t+1} = \begin{bmatrix} x_{t+1} \\ d_{t+1} \end{bmatrix} = \underbrace{\begin{bmatrix} f(x_t, u_t + d_t) \\ d_t \end{bmatrix}}_{h(\mathcal{X}_t, u_t)} + \underbrace{\begin{bmatrix} w_t \\ s_t \end{bmatrix}}_{n_t}, \tag{4.95}$$

$$y_t = \underbrace{g(M\mathcal{X}_t)}_{g_e(\mathcal{X}_t)} + v_t. \tag{4.96}$$

where $M = \begin{bmatrix} I & 0 \end{bmatrix}$ and $n_t \sim \mathcal{N}(n_t; 0, Q) = \text{diag}\{Q, \rho^2\}$ and ρ being a small positive constant. The extended model used to estimate the system states and disturbances is given by:

$$\mathcal{X}_{t+1} = h(\mathcal{X}_t, u_t) + n_t, \tag{4.97}$$

$$y_t = g_e(\mathcal{X}_t) + v_t, \tag{4.98}$$

where n_t and v_t represent process and measurement noise, respectively.

Within this estimation framework, we can effectively model the discrepancies between the AM2 and ADM1 models. This allows the estimation of the disturbance $\hat{d}_{t|t}$, which facilitates compensation through the control action and enables precise reference tracking. Consequently, the control signal at the current time step is expressed as:

$$u_t = u_{t-1} + \delta u_0^* + \hat{d}_{t|t}. \tag{4.99}$$

This approach ensures that the integral action effectively reduces steady state error, thereby enhancing the robustness and accuracy of the control system in managing the anaerobic digestion process.

4.5. Final Control Strategy

The implemented control system integrates two advanced techniques: the Extended Kalman Filter (EKF) for state estimation and the Nonlinear Model Predictive Control (NMPC) for optimal control. This strategy leverages the EKF to enhance the accuracy of state measurements and the NMPC to ensure control actions, even in the presence of nonlinear dynamics and disturbances.

The process begins with system measurements, which are processed by the EKF. Using a extended system model $h(\mathcal{X}_t, u_t)$ with the extended state vector $\mathcal{X}_t = \begin{bmatrix} x_t & d_t \end{bmatrix}^T$, the EKF provides estimates for both the states of the AM2 model and the disturbance term $\hat{d}_{t|t}$. This estimation process can be represented by the following extended system:

$$\mathcal{X}_{t+1} = h(\mathcal{X}_t, u_t) + n_t, \tag{4.100}$$

$$y_t = g_e(\mathcal{X}_t) + v_t, \tag{4.101}$$

Once the state estimates are obtained, they are used to define the NMPC optimization problem. This problem is formulated to minimize a cost function that penalizes deviations from the desired system output as well as excessive control effort:

$$J = \min_{\delta u_0,\ldots,\delta u_{N-1}} ||y_t - y_{\text{ref}}||_Q^2 + ||\delta u_t||_R^2 \tag{4.102}$$

$$\text{s.t.} \quad x_{t+1} = f(x_t, u_t), \quad t \geq 0 \tag{4.103}$$

$$y_t = g(x_t, u_t), \quad t \geq 0 \tag{4.104}$$

$$x_t \in \mathcal{X}, \quad u_t \in \mathcal{U}, \quad t = 0, ..., N-1 \tag{4.105}$$

$$x_N \in \mathcal{X}_f \tag{4.106}$$

$$u_t = u_{t-1} + \delta u_t + \hat{d}_{t|t}, \quad t \geq 0 \tag{4.107}$$

$$x_0 = \hat{x}_{t|t} \tag{4.108}$$

$$u_{\min} \leq u_t \leq u_{\max} \tag{4.109}$$

$$\delta u_{\min} \leq \delta u_t \leq \delta u_{\max}, \tag{4.110}$$

Finally, after solving the optimization problem, the first optimal control action, δu_t, is applied to the system, updating the control input as follows:

$$u_t = \delta u_0^* + u_{t-1}. \tag{4.111}$$

This combined approach ensures robust control performance, addressing uncertainties through the EKF and achieving optimal operation via NMPC.

5. Results

This section presents the outcomes of implementing the tools developed in the preceding chapters to effectively control the anaerobic digestion process, utilizing the ADM1 simulator as the source of real data.

The final control diagram implemented for the system is illustrated in Figure 5.14. In this diagram, the Extended Kalman Filter (EKF) serves as the state estimator, receiving inputs from the measurement y_t and the control signal u_t. The EKF employs an extended state vector, which facilitates the estimation of both the state values and a disturbance $\hat{d}_{t|t}$. These estimates are subsequently fed into the Nonlinear Model Predictive Controller (NMPC), which incorporates integral action and leverages the AM2 model to compute the optimal control signal. This control signal is then applied to the ADM1 plant to effectively track the desired reference trajectory.

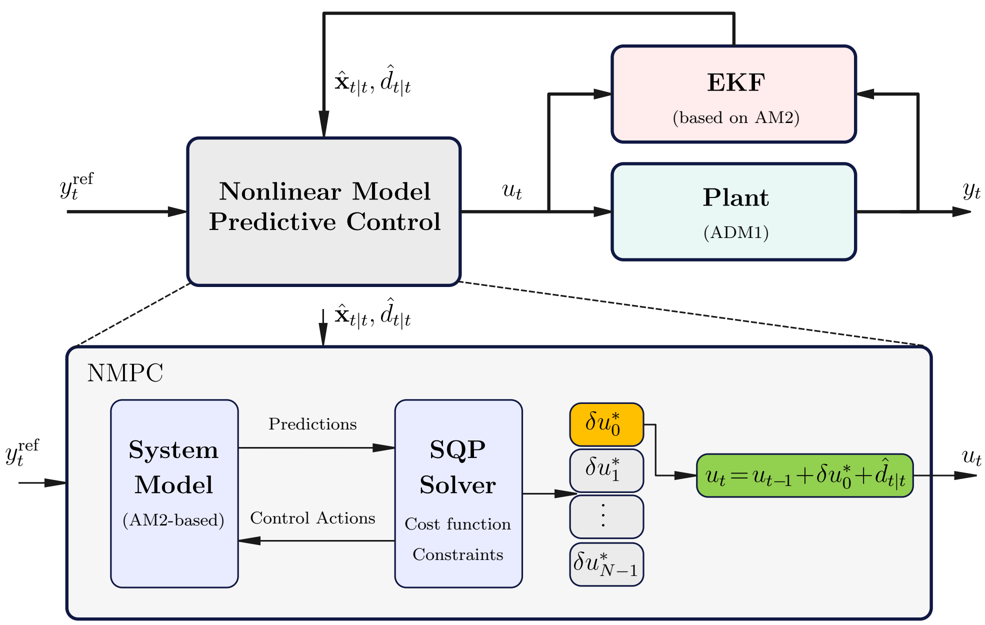

Figure 5.14: Schematic of EKF-NMPC framework implemented

5.1. Simulation

For this simulation, the same scenario used in the previous sections was considered, which corresponds to a 20 days simulation with four reference signals changing every five days. Additionally, measurement noise was included in the system to assess the robustness of the controller under realistic operating conditions. For this purpose, white noise with a mean of 0 and a standard deviation of 0.1 was utilized, simulating the inherent uncertainties that can occur in practical systems.

Figures 5.15, 5.16, and 5.17 present the results of the simulation, corresponding to the output, input, and reference tracking error plots, respectively. These graphs illustrate how the system responds under the influence of measurement noise, as well as the differences between the models used and how the NMPC controller in conjunction with the EKF manages to stabilize the system effectively.

In the early stages of the simulation, it is observed that the controller and estimator do not function correctly due to initial conditions differing from the actual system conditions. This phenomenon is common in control systems and is referred to as the "initial condition problem." However, after a few sampling cycles, by day 1 of the simulation, the system stabilizes, achieving errors below 2%. The rapid convergence indicates the effectiveness of the NMPC strategy in adapting to changing conditions.

For the subsequent reference setpoints, it can be observed that during these abrupt changes, the error spikes to a significant value. This behavior is expected during transient phases when the system is adjusting to new reference values. Nonetheless, the integral action implemented in the controller works effectively to reduce the error to a value close to 0. This is evident in Figure 5.16, where it is seen that for higher desired reference values, the estimator detects this error and increases the estimated disturbance $\hat{d}_{t|t}$ to compensate for the difference between the models. This adaptive capability allows the controller to manage disturbances robustly and accurately, ensuring the system's stability.

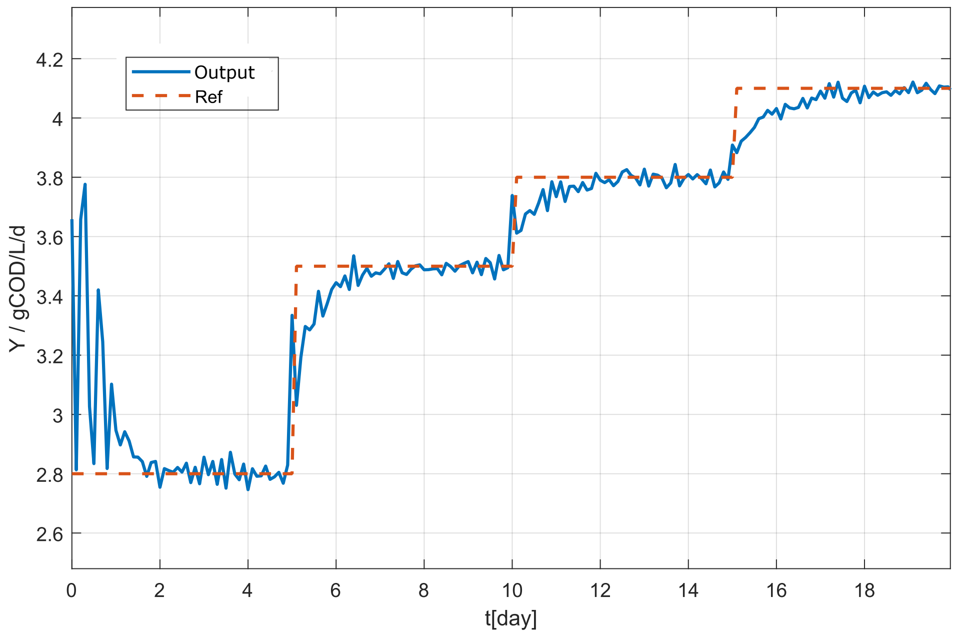

Figure 5.15: Final Simulation: Output Signal Plot

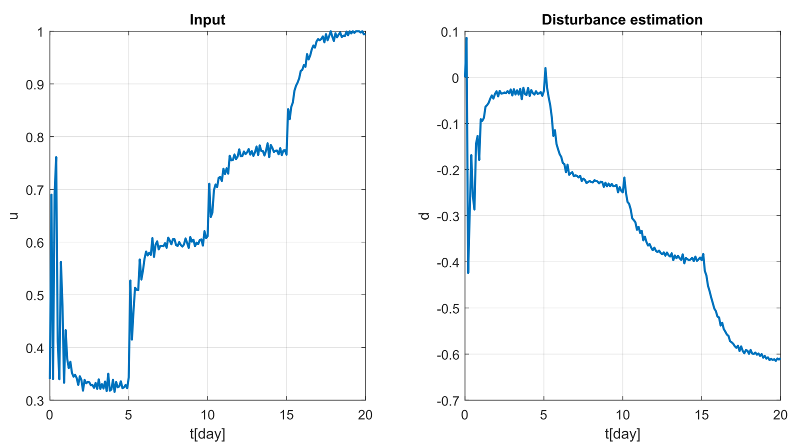

Figure 5.16: Final Simulation: Input Signal and Disturbance Estimation Plot

5.2. Analysis of Different Scenarios

To validate the implementations developed during this thesis, several performance metrics were utilized, including RMSE (Root Mean Square Error), MAPE (Mean Absolute Percentage Error), and the maximum error. These metrics provide insights into the accuracy and reliability of the control strategies implemented and allow for an objective comparison between different approaches.

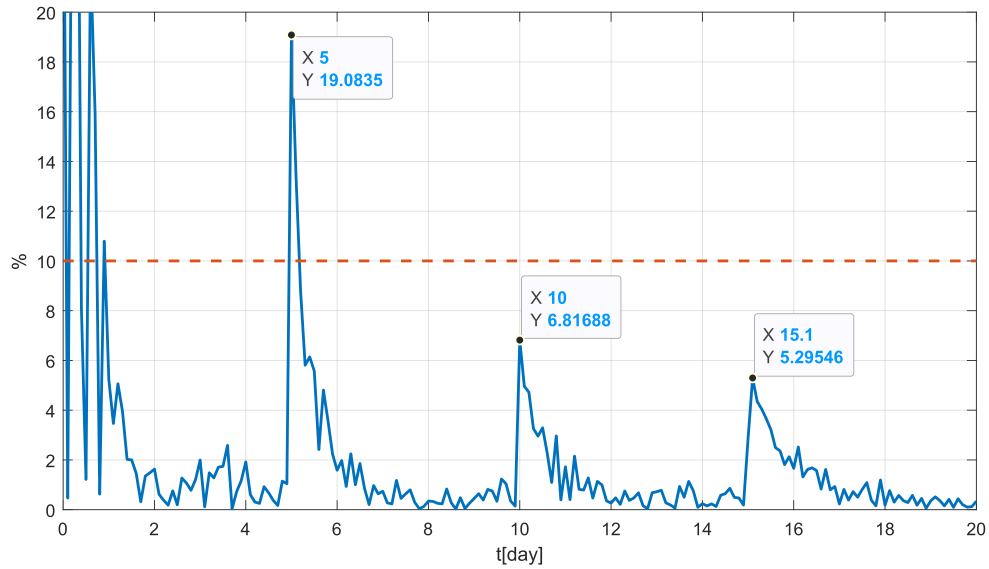

Figure 5.17: Final Simulation: Reference Tracking Error Plot

For these analyses, simulations were conducted for the following cases:

- Case 1: Previous paper, NMPC assuming measurements of the entire process.
- Case 2: NMPC + EKF.
- Case 3: NMPC + EKF + Parameter Identification.
- Case 4: NMPC + EKF + Integration.
- Case 5: NMPC + EKF + Parameter Identification + Integration.
- Case 6: NMPC + EKF + Parameter Identification + Integration + Measurement Noise.

In each case, the scenario used in previous simulations was replicated, but the control strategy was altered to evaluate the impact of each method. The metrics calculated for each simulation assessed the accuracy and efficiency of each combination of implemented methods. This systematic approach ensures that the obtained results can be clearly compared, highlighting the strengths and weaknesses of each configuration under varying operational conditions. The results can be found in Tables 5.4 and 5.5, where the metrics related to reference tracking error are presented. **For additional details and analyses of the remaining cases, please refer to the appendix.**

Case	RMSE	MAPE	Max Error
1	0.1801	4.6445	17.9121
2	0.3590	8.1372	15.4087
3	0.2322	4.8303	19.2332
4	0.1265	2.5705	15.8027
5	0.1390	1.9106	33.0463
6	0.1503	2.1122	34.8687

Table 5.4: Analysis of Each Control Strategy

Case	Segment 1	Segment 2	Segment 3	Segment 4
1	3.7479	5.3455	4.7394	4.7431
2	1.5770	8.3637	10.0399	12.4814
3	2.1744	7.7770	8.8259	0.6280
4	5.3408	2.2865	1.1708	1.5051
5	3.5706	1.7855	1.0455	1.2540
6	4.2024	1.9621	1.1286	1.1742

Table 5.5: Percentage Errors Relative to Each Reference Segment

Based on the results obtained from implementing different control strategies, it can be concluded that the best strategy is the one that integrates both state estimation and integral action (Case 5). This is reflected in Table 5.4, where lower RMSE and MAPE values were obtained, indicating a more accurate tracking of the reference signals. Although there may be higher errors in this case, they occur only during the transient period and for a brief time, during which the state estimator converges to values that stabilize the system. This effect is evident in Table 5.5, where segment 1 shows a higher error compared to the other segments, but in the following segments, the errors are significantly reduced and stabilize to a value close to 1%. If this peak error is a concern, it can be easily addressed by incorporating a low-pass filter into the reference signal to smooth out rapid changes and avoid sharp peaks in the tracking error.

Regarding Case 5 and Case 6, the latter includes measurement noise in the system. Despite this disturbance, it can be seen that the metrics obtained in both cases are similar, demonstrating the robustness of the implemented control strategy. This indicates that the filtering component functions correctly, allowing the controller to effectively follow the desired reference even under noisy conditions. The ability to maintain performance in the presence of measurement noise is a critical advantage for practical applications, as real-world systems often experience such disturbances.

In summary, the integration of state estimation and control strategies significantly enhances the performance of the NMPC framework. The results affirm the importance of adaptive mechanisms, such as EKF and integral action, in managing uncertainties and improving system stability. Future work may explore additional filtering techniques and their effects on system performance, as well as the implementation of this framework in real-time applications, to further validate its effectiveness in practical scenarios.

6. Conclusions

Throughout this thesis, the feasibility and potential of an advanced control scheme integrating Nonlinear Model Predictive Control (NMPC) and Extended Kalman Filters (EKF) for effective management of the anaerobic digestion process modeled by ADM1 have been demonstrated. The research focused on addressing the inherent complexities and nonlinearities associated with the anaerobic digestion process, providing valuable insights into how these challenges can be met with sophisticated control techniques.

The following key points were validated during this work:

- A successful NMPC-EKF control scheme was developed and implemented to address the challenges of the nonlinear nature and variability of the ADM1 process using AM2 as the main model. This hybrid approach effectively leveraged the predictive capabilities of NMPC while simultaneously employing EKF for state estimation, resulting in a robust control strategy tailored for the dynamic characteristics of anaerobic digestion.

- The proposed control strategies were evaluated in realistic scenarios with changes in reference signals, demonstrating precise tracking of desired references. The transition from an ideal (non-implementable) scheme to an NMPC-EKF scheme, which is feasible for real plants, resulted in improvements of 22.82% in RMSE and 58.86% in MAPE. These improvements highlight the effectiveness of the proposed methods in achieving better control performance compared to conventional strategies, emphasizing the practical applicability of NMPC-EKF in real-world scenarios.

- A complementary integration technique was implemented in addition to the NMPC scheme, allowing compensation for the error between the two models used in the simulations. This led to a reduction in steady-state errors from 12% to values below 1%. The integration technique not only enhanced accuracy but also contributed to overall system stability, ensuring that the control system could maintain optimal performance even in the face of disturbances and uncertainties.

- Codes were developed and the process was documented to facilitate future implementations in a real plant. This aspect of the work is crucial as it paves the way for practical applications of the research findings, ensuring that the developed control strategies can be effectively translated into operational environments, thereby enhancing the viability of implementing advanced control methodologies in the field of anaerobic digestion.

In conclusion, the integration of NMPC and EKF presents a promising approach for the advanced control of anaerobic digestion processes, addressing key challenges related to non-linearity and variability. The findings of this thesis not only contribute to the theoretical understanding of control systems in this context but also provide a practical framework for implementation in real-world applications. Future research may explore the integration of additional advanced techniques, such as reinforcement learning or adaptive control, to further enhance the adaptability and efficiency of control strategies in dynamic environments. Overall, this work lays the foundation for future advancements in the field of process control, particularly in renewable energy systems such as anaerobic digestion.

6.1. Future Work

After implementing the control system and ensuring its proper functionality, the following areas for future work have been identified:

- Accelerate the process of obtaining the optimal control signal: Simulating the process over an extended period in MATLAB is time-consuming. The bottleneck in the implemented code is the NMPC block that solves the optimization problem. It is proposed to replace the NMPC block with a neural network, which would act as an NMPC controller, thereby reducing computation time.

- Diversify the types of waste in the anaerobic digestion process: In this thesis, simulations were performed with the process configured for wine waste. It is suggested to implement the control system for different types of waste, thereby expanding its applicability.

- Improve the AM2 model: It is recommended to develop algorithms that allow for adjusting all parameters of the AM2 model or even obtaining an improved version of the anaerobic digestion process. This would enable the control system to manage the process efficiently, regardless of the type of waste.

7. Appendix

7.1. Simulations

In this annex, the images corresponding to the simulations performed for the case presented in the results chapter. These simulations illustrate the behavior of the system under the proposed control and estimation methods. Specifically, the output signals with the reference will be plotted, along with the input signal and the error between the output and the reference. The analysis of these results will provide a better understanding of the system's performance and highlight any potential areas for improvement.

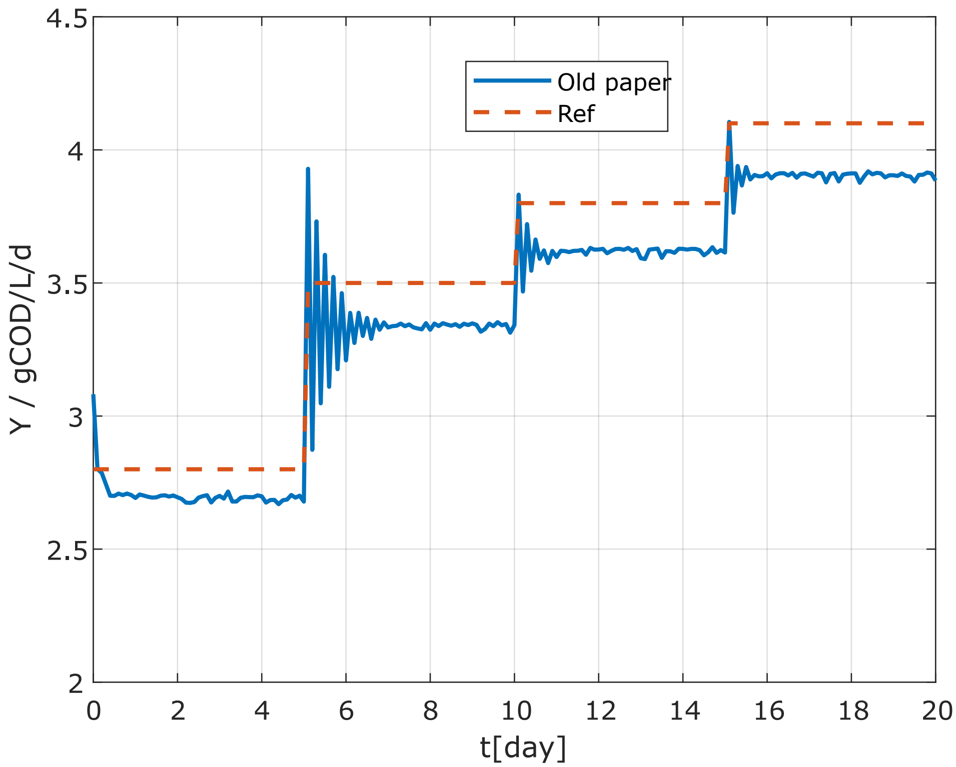

Figure 7.18: Case 1: Output Signal Plot

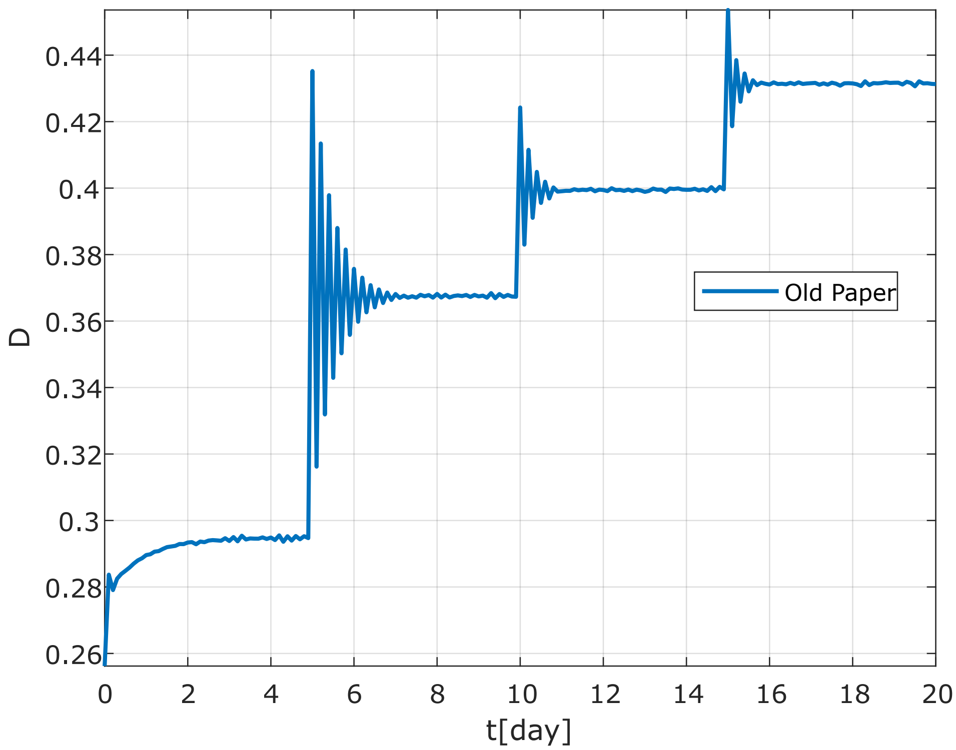

Figure 7.19: Case 1: Input Signal Plot

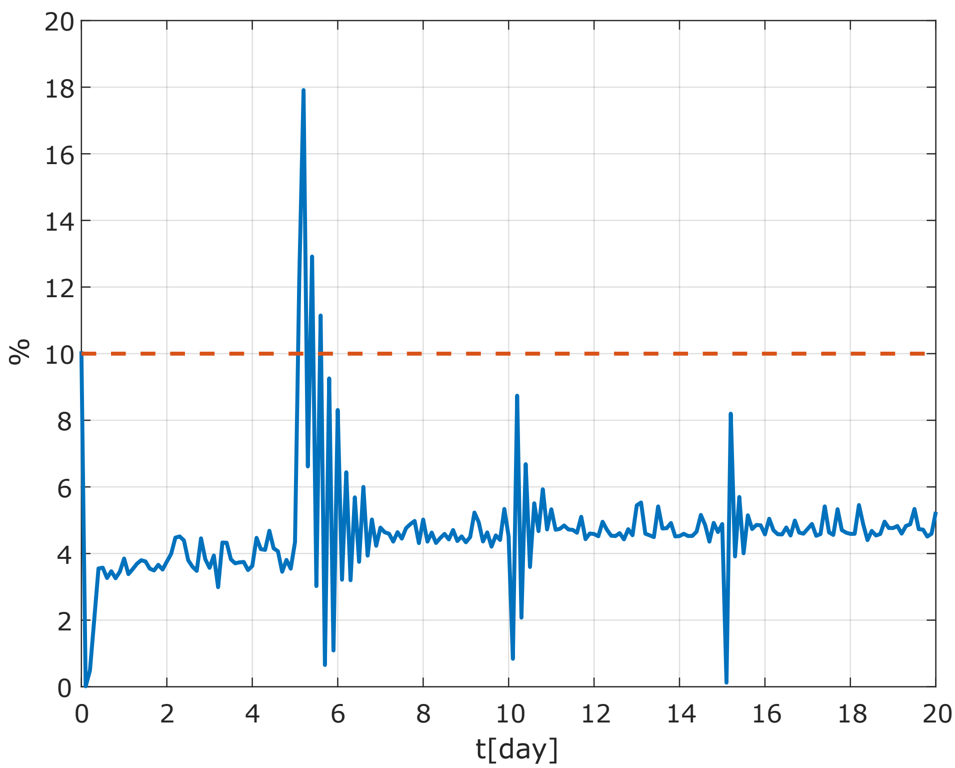

Figure 7.20: Case 1: Reference Tracking Error Plot

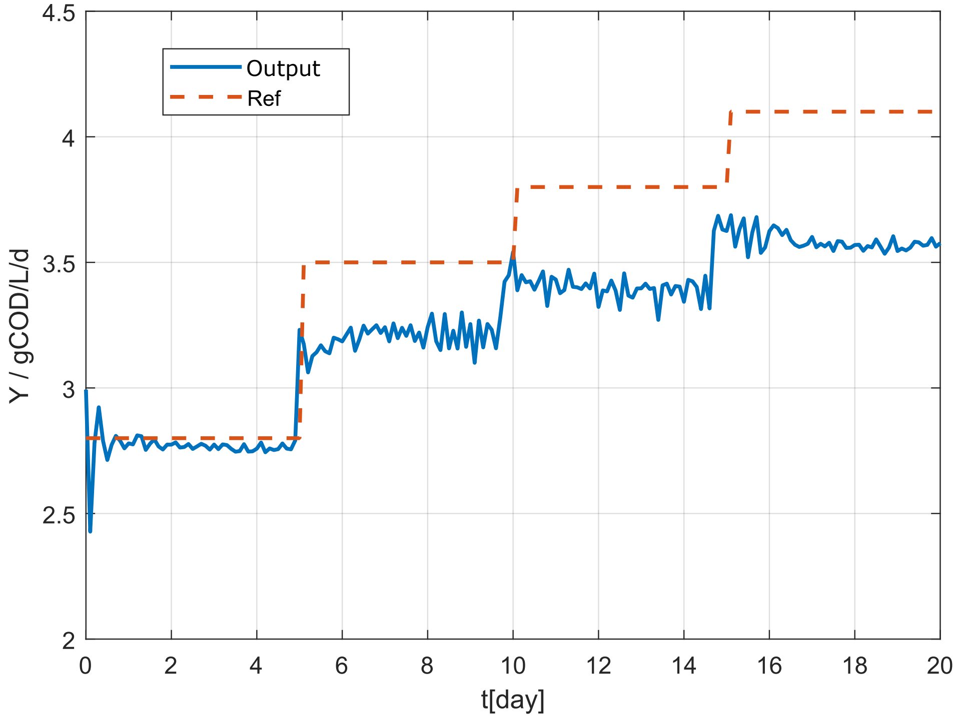

Figure 7.21: Case 2: Output Signal Plot

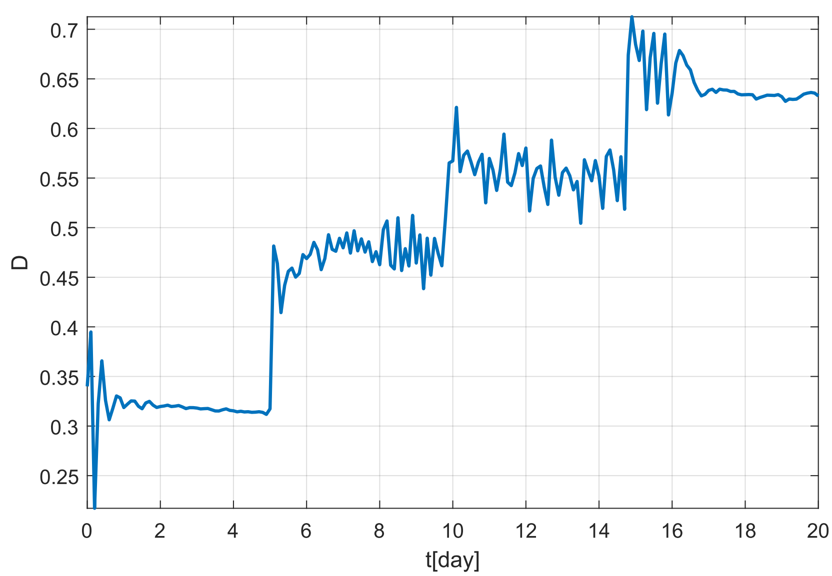

Figure 7.22: Case 2: Input Signal Plot

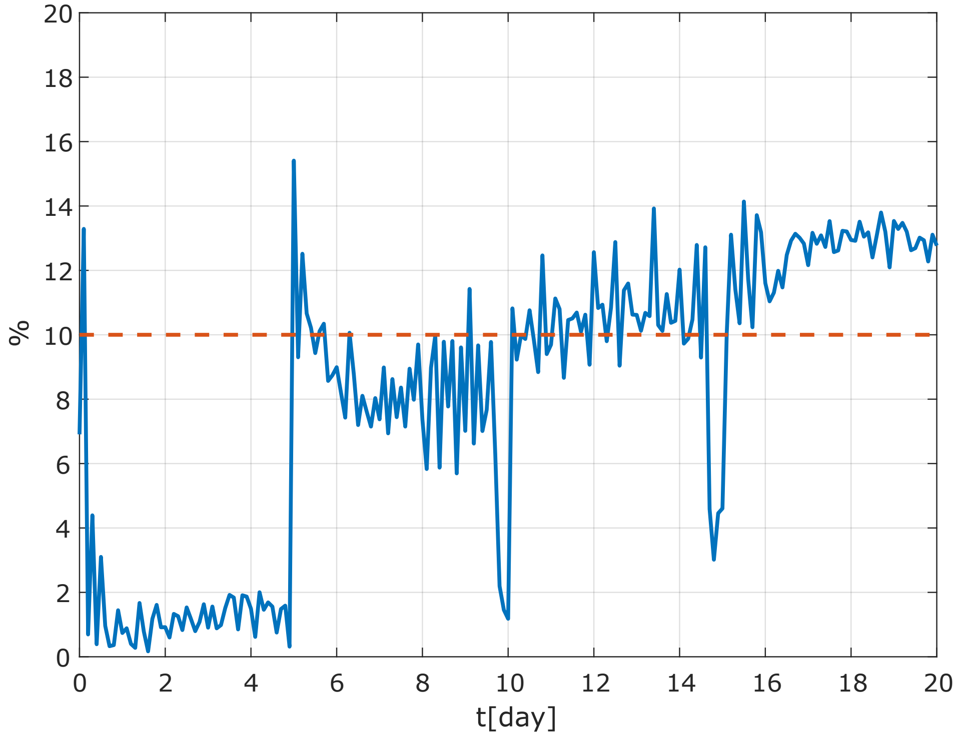

Figure 7.23: Case 2: Reference Tracking Error Plot

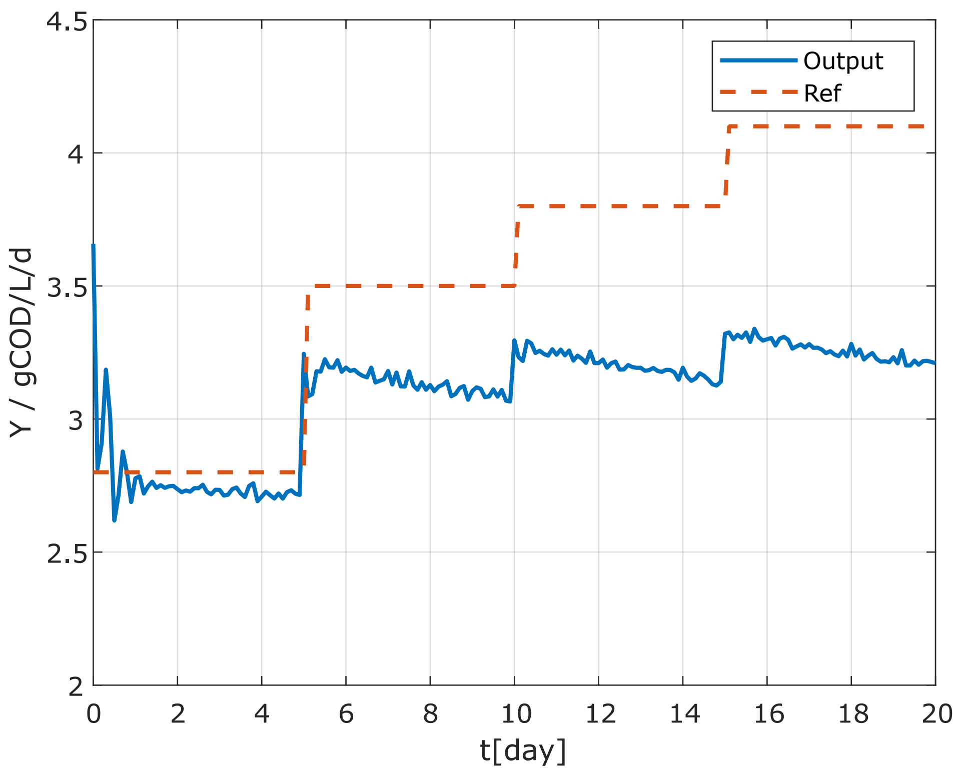

Figure 7.24: Case 3: Output Signal Plot

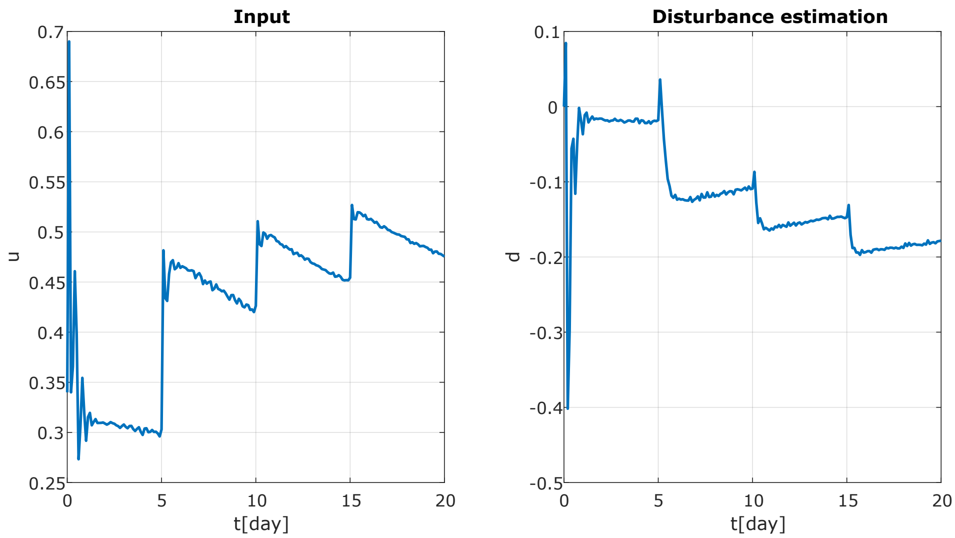

Figure 7.25: Case 3: Input Signal and Disturbance Estimation Plot

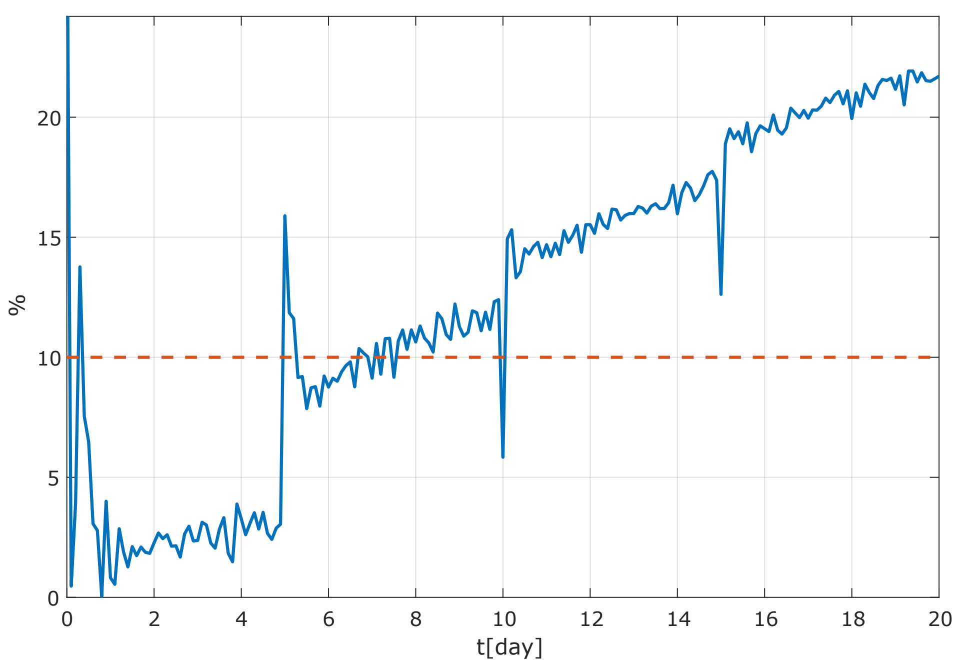

Figure 7.26: Case 3: Reference Tracking Error Plot

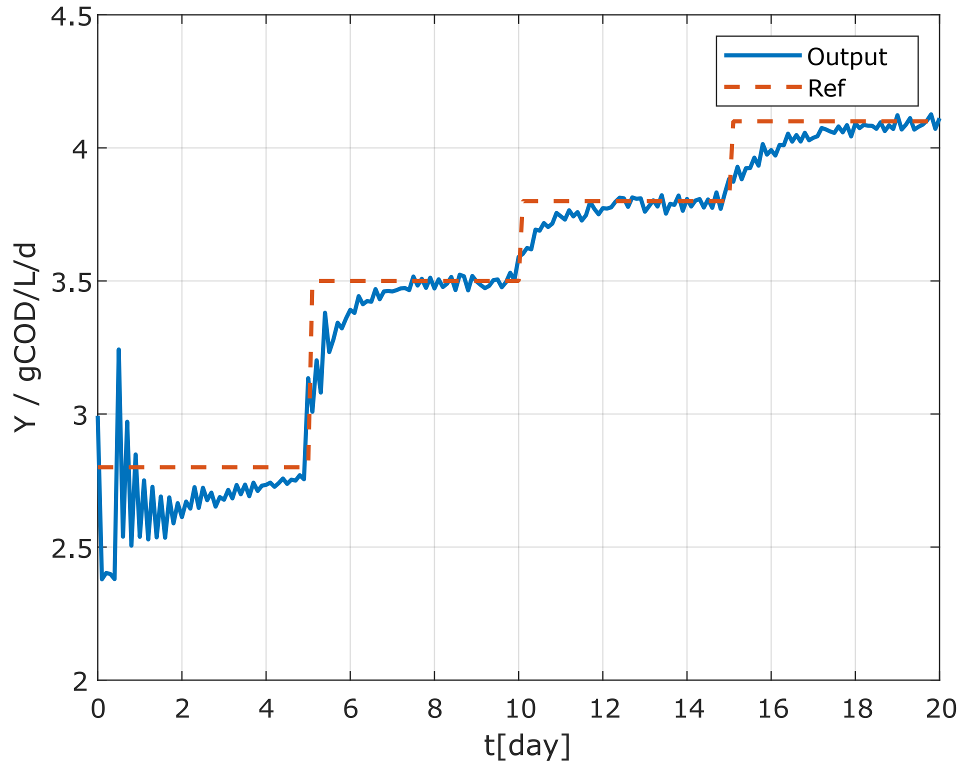

Figure 7.27: Case 4: Output Signal Plot

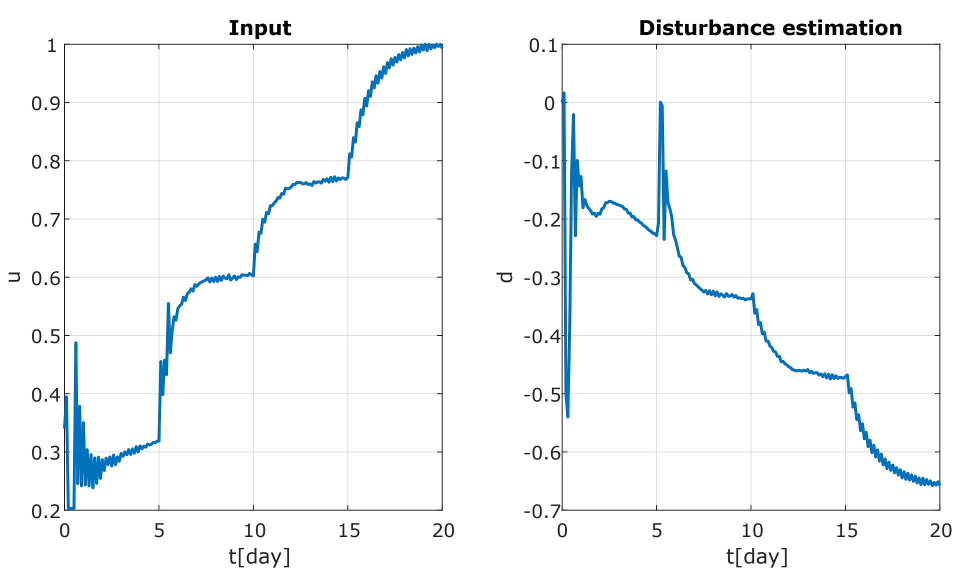

Figure 7.28: Case 4: Input Signal and Disturbance Estimation Plot

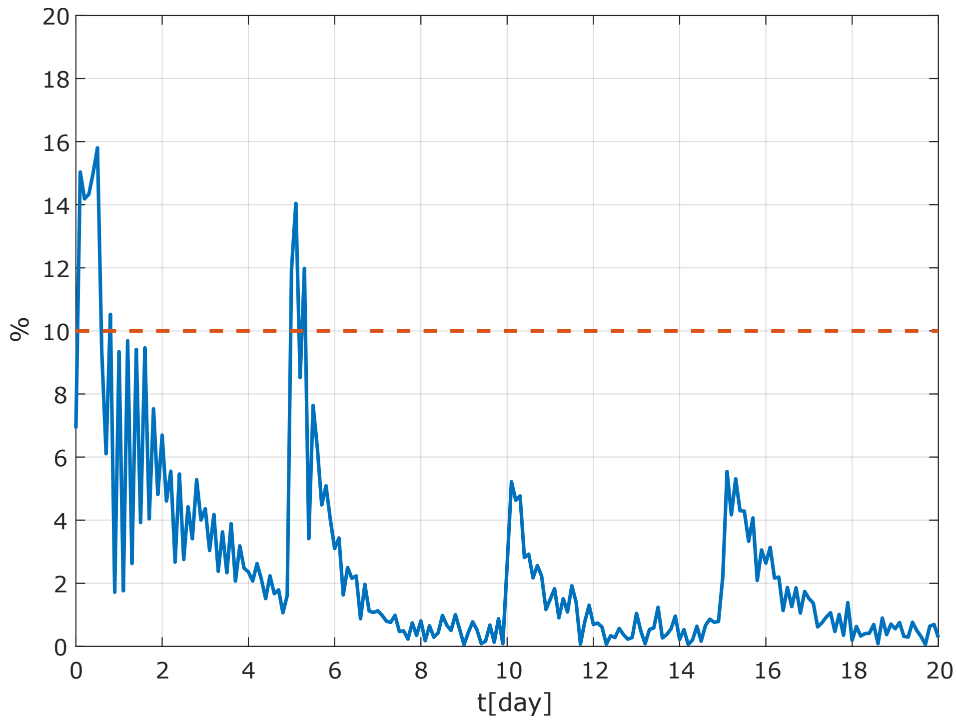

Figure 7.29: Case 4: Reference Tracking Error Plot

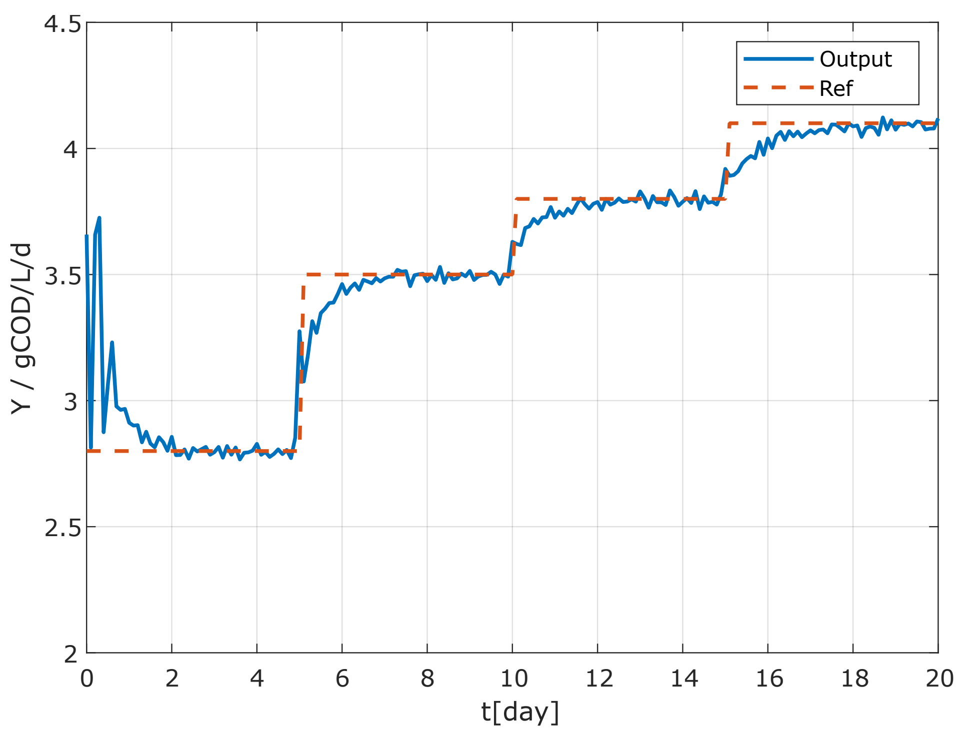

Figure 7.30: Case 5: Output Signal Plot

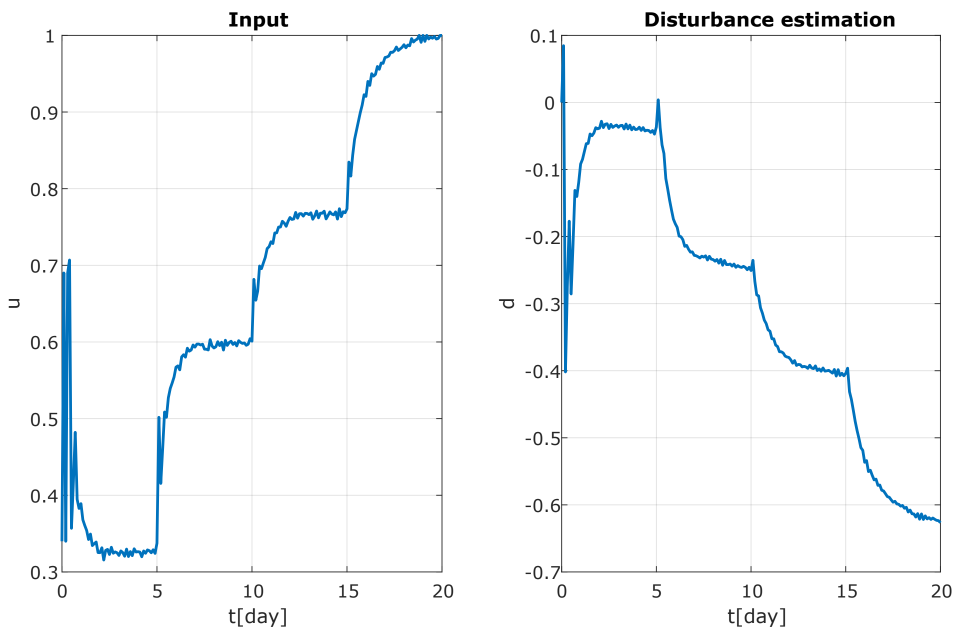

Figure 7.31: Case 5: Input Signal and Disturbance Estimation Plot

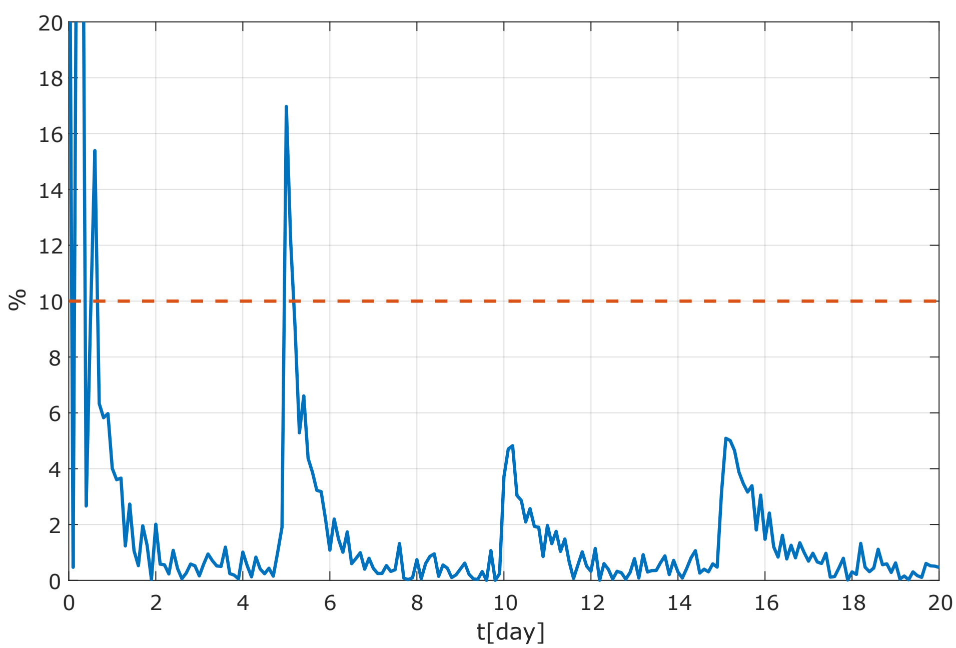

Figure 7.32: Case 5: Reference Tracking Error Plot

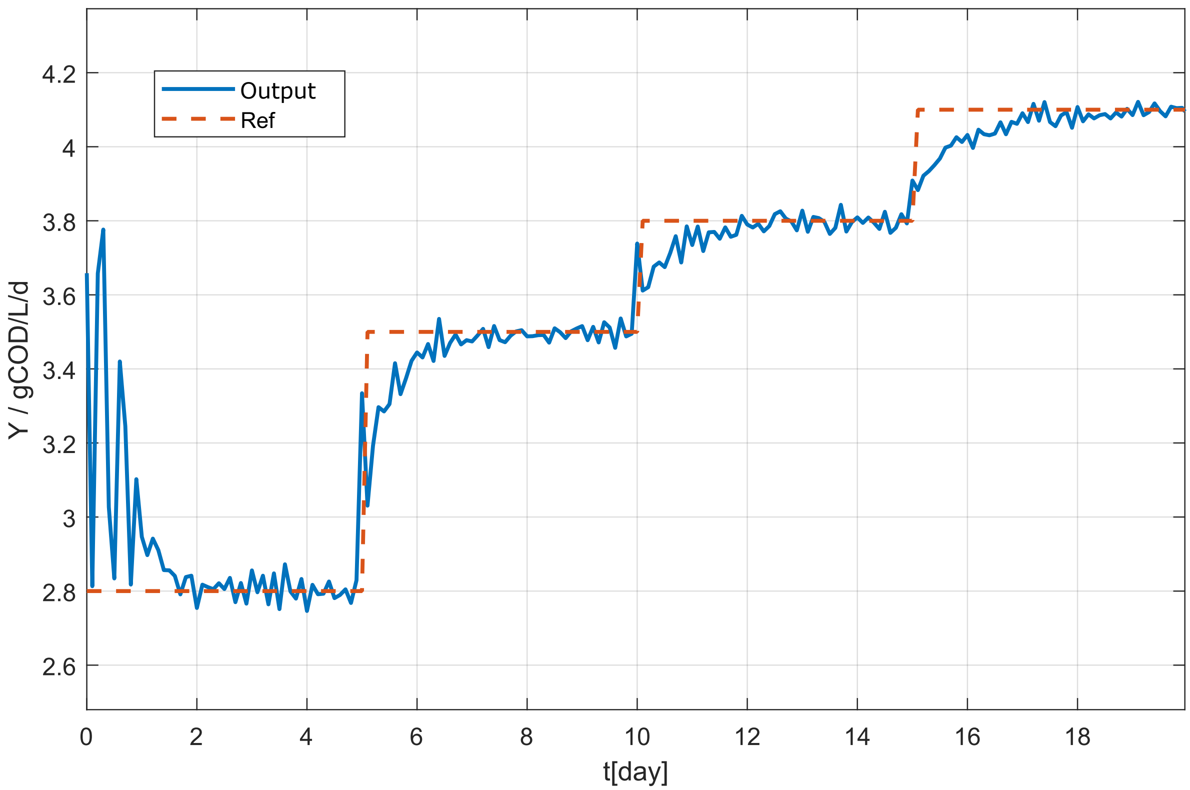

Figure 7.33: Case 6: Output Signal Plot

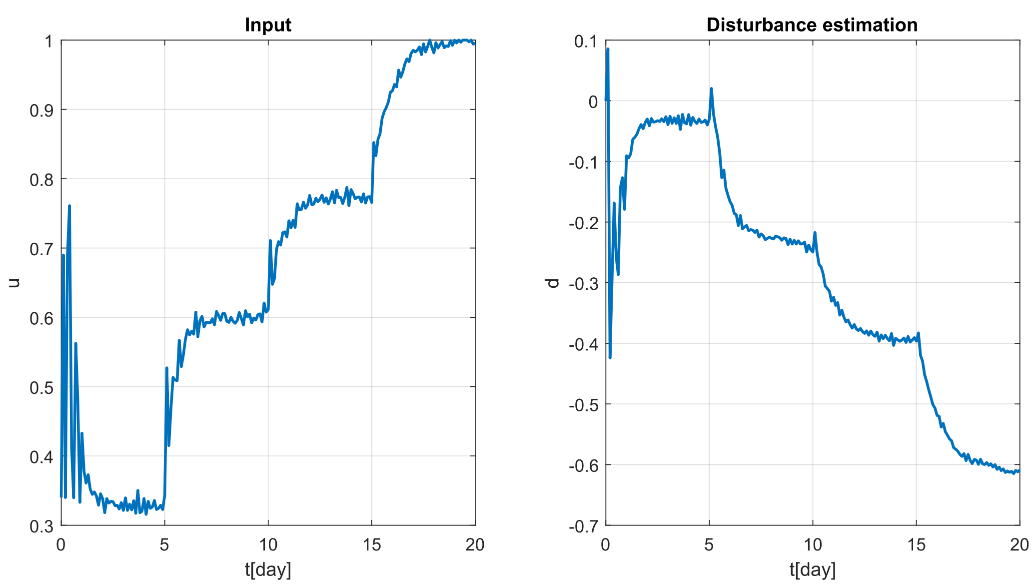

Figure 7.34: Case 6: Input Signal and Disturbance Estimation Plot

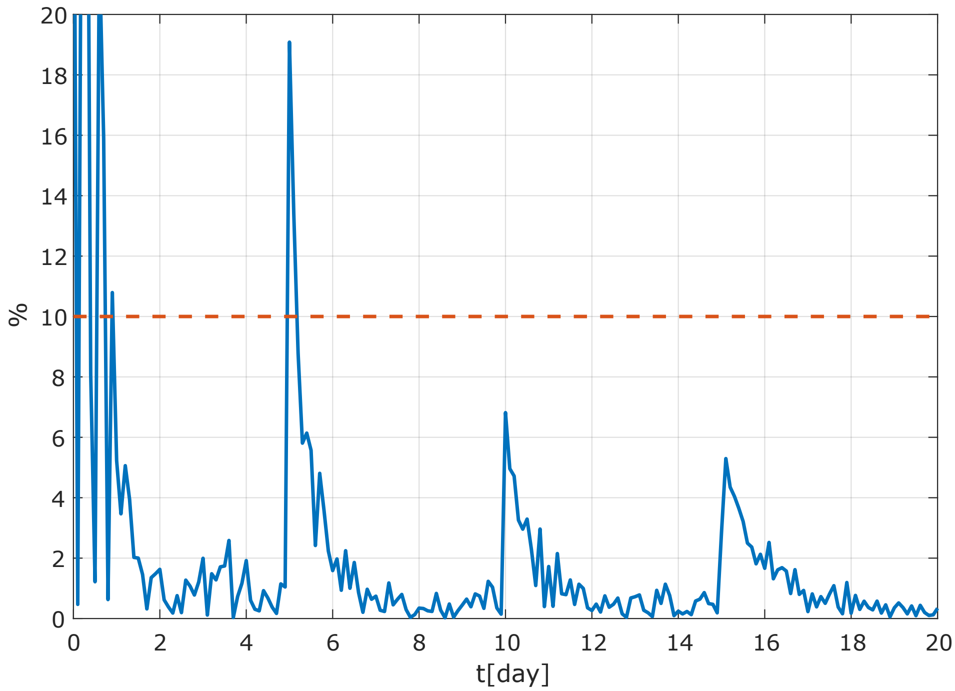

Figure 7.35: Case 6: Reference Tracking Error Plot

References

[1] G. Sánchez, *Digestión Anaerobia (serie)*, ser. Folleto técnico / UADY. Universidad Autónoma de Yucatán, 1996. [Online]. Available: https://books.google.cl/books?id=1Sxpl-0KBgoC

[2] I. Angelidaki, L. Treu, P. Tsapekos, G. Luo, S. Campanaro, H. Wenzel, and P. G. Kougias, "Biogas upgrading and utilization: Current status and perspectives," *Biotechnology advances*, vol. 36, no. 2, pp. 452–466, 2018.

[3] Y. Chen, J. J. Cheng, and K. S. Creamer, "Inhibition of anaerobic digestion process: a review," *Bioresource technology*, vol. 99, no. 10, pp. 4044–4064, 2008.

[4] S. García-Gen, J. M. Lema, and J. Rogríguez, "Generalised modelling approach for anaerobic co-digestion of fermentable substrates," *Bioresource Technology*, vol. 147, pp. 525–533, 2013.

[5] J. Jimenez, E. Latrille, J. Harmand, A. Robles, J. Ferrer, D. Gaida, C. Wolf, F. Mairet, O. Bernard, V. Alcaraz-Gonzalez *et al.*, "Instrumentation and control of anaerobic digestion processes: a review and some research challenges," *Reviews in Environmental Science and Bio/Technology*, vol. 14, pp. 615–648, 2015.

[6] L. Wang, *Model predictive control system design and implementation using MATLAB®*. Springer Science & Business Media, 2009.

[7] L. Condrachi and M. Barbu, "Anaerobic digestion processes controller tuning using fictitious reference iterative method," *IFAC-PapersOnLine*, vol. 55, no. 7, pp. 453–458, 2022.

[8] D. J. Batstone, D. Puyol, X. Flores-Alsina, and J. Rodríguez, "Mathematical modelling of anaerobic digestion processes: applications and future needs," *Reviews in Environmental Science and Bio/Technology*, vol. 14, pp. 595–613, 2015.

[9] D. Nguyen, V. Gadhamshetty, S. Nitayavardhana, and S. K. Khanal, "Automatic process control in anaerobic digestion technology: A critical review," *Bioresource Technology*, vol. 193, pp. 513–522, 2015. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S0960852415008718

[10] S. García-Gen, J. Rodríguez, and J. M. Lema, "Optimisation of substrate blends in anaerobic co-digestion using adaptive linear programming," *Bioresource Technology*, vol. 173, pp. 159–167, 2014.

[11] R. Mo, W. Guo, D. Batstone, J. Makinia, and Y. Li, "Modifications to the anaerobic digestion model no. 1 (adm1) for enhanced understanding and application of the anaerobic treatment processes – a comprehensive review," *Water Research*, vol. 244, p. 120504, 2023. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S0043135423009442

[12] L. F. Núñez Pintado, "Modelamiento y control de proceso de digestión anaerobia para la producción de biogás a partir de residuos orgánicos y/o aguas residuales," 2017.

[13] S. Attar and F. Haugen, "Comparison of different state estimator algorithms applied to a simulated anaerobic digestion reactor," in *Linköping Electronic Conference Proceedings*, 2018, pp. 118–125.

[14] N. Raeyatdoost, M. Bongards, T. Bäck, and C. Wolf, "Robust state estimation of the anaerobic digestion process for municipal organic waste using an unscented kalman filter," *Journal of Process Control*, vol. 121, pp. 50–59, 2023. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S0959152422002153

[15] A. Doucet, S. Godsill, and C. Andrieu, "On sequential monte carlo sampling methods for bayesian filtering," *Statistics and computing*, vol. 10, no. 3, pp. 197–208, 2000.

[16] N. J. Gordon, D. J. Salmond, and A. F. M. Smith, "Novel approach to nonlinear/non-gaussian bayesian state estimation," *IEE Proceedings F - Radar and Signal Processing*, vol. 140, no. 2, pp. 107–113, 1993.

[17] S. García-Gen, J. Rodríguez, and J. M. Lema, "Control strategy for maximum anaerobic co-digestion performance," *Water research*, vol. 80, pp. 209–216, 2015.

[18] L. Xue, D. Li, and Y. Xi, "Nonlinear model predictive control of anaerobic digestion process based on reduced adm1," in *2015 10th Asian Control Conference (ASCC)*, 2015, pp. 1–6.

[19] H. Xie, L. Dai, Y. Lu, and Y. Xia, "Disturbance rejection mpc framework for input-affine nonlinear systems," *IEEE Transactions on Automatic Control*, vol. 67, no. 12, pp. 6595–6610, 2022.

[20] I. A. Jimoh, "A novel approach to disturbance rejection in constrained model predictive control," *arXiv preprint arXiv:2103.09865*, 2021.

[21] S. García-Gen, L. O. Santos, and A. V. Wouwer, "Application of a nonlinear model predictive controller to the anaerobic digestion of readily biodegradable wastes," *IFAC-PapersOnLine*, vol. 55, no. 7, pp. 909–914, 2022.

[22] R. E. Kalman, "A new approach to linear filtering and prediction problems," *Journal of Fluids Engineering, Transactions of the ASME*, vol. 82, no. 1, pp. 35–45, 1960.

[23] D. Pan, H. Li, and Y. Song, "A comparative study of particle filters and its variants in lithium-ion battery soh estimation," in *2020 International Conference on Sensing, Measurement & Data Analytics in the era of Artificial Intelligence (ICSMD)*. IEEE, 2020, pp. 198–203.

[24] J. B. Rawlings, D. Q. Mayne, and M. Diehl, *Model predictive control: theory, computation, and design*. Nob Hill Publishing Madison, 2017, vol. 2.

[25] F. Borrelli, A. Bemporad, and M. Morari, *Predictive control for linear and hybrid systems*. Cambridge University Press, 2017.

[26] T. Albin Rajasingham, "Formulation of the optimization problem," in *Nonlinear Model Predictive Control of Combustion Engines: From Fundamentals to Applications.* Springer, 2021, pp. 139–172.

[27] D. J. Batstone, J. Keller, I. Angelidaki, S. V. Kalyuzhnyi, S. G. Pavlostathis, A. Rozzi, W. Sanders, H. Siegrist, and V. A. Vavilin, "The iwa anaerobic digestion model no 1 (adm1)," *Water Science and technology*, vol. 45, no. 10, pp. 65–73, 2002.

[28] F. Blumensaat and J. Keller, "Modelling of two-stage anaerobic digestion using the iwa anaerobic digestion model no. 1 (adm1)," *Water Research*, vol. 39, no. 1, pp. 171–183, 2005.

[29] B. C. B. Benyahia, T. Sari and J. Harmand, "Bifurcation and stability analysis of a two step model for monitoring anaerobic digestion processes," *Journal of Process Control*, vol. 22, no. 6, pp. 1008–1019, 2012. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S0959152412000972

[30] B. Benyahia, T. Sari, B. Cherki, and J. Harmand, "Bifurcation and stability analysis of a two step model for monitoring anaerobic digestion processes," *Journal of Process Control*, vol. 22, no. 6, pp. 1008–1019, 2012. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S0959152412000972

[31] S. García-Gen, L. O. Santos, and A. V. Wouwer, "Application of a nonlinear model predictive controller to the anaerobic digestion of readily biodegradable wastes," *IFAC-PapersOnLine*, vol. 55, no. 7, pp. 909–914, 2022.

[32] M. Azúa-Poblete, A. L. Cedeño, S. García-Gen, and J. C. Agüuero, "On state estimation methods for an anaerobic digestion model for readily biodegradable substrates," in *2023 IEEE CHILEAN Conference on Electrical, Electronics Engineering, Information and Communication Technologies (CHILECON).* IEEE, 2023, pp. 1–6.

[33] T. Söderström, *Discrete-Time Stochastic Systems Estimation and Control.* Springer Science & Business Media, 2002.