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Data-Driven Modelling of Biogas Production Using Multi-Task Gaussian Processes

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ABSTRACT

This study introduces the novel application of a Multi-Task Gaussian Process (MTGP) model to predict biogas production and critical anaerobic digestion (AD) performance indicators (soluble COD, volatile fatty acids (VFAs)), addressing feedstock variability and dynamic process behavior. We compare the MTGP against the widely used mechanistic AM2 model to evaluate its accuracy and applicability for probabilistic modeling in AD systems. The MTGP framework leverages multi-output correlations and uncertainty quantification, trained on experimental data, achieving superior predictive performance over AM2in this study, with lower RMSE (SCOD: 0.32 g/L; VFAs: 0.87 mmol/L; biogas: 0.15 L/day) and higher R^2 values (SCOD:0.91, VFAs:0.94, biogas :0.88) under the conditions tested. While AM2 provides biochemical insights, its reliance on unvalidated assumptions may limits robustness. The flexibility of MTGP and precision suggest its potential for real-world applications such as Bayesian Optimization and Design of Experiments, enabling data-driven process enhancement without mechanistic constraints. This work establishes MTGP as a pioneering tool for AD optimization, bridging data-driven efficiency with practical bioenergy challenges.

Keywords: Anaerobic Digestion, Biogas Production, Multi-Task Gaussian Process, Data-driven Modelling, Mechanistic Modeling, Predictive Analytics.

INTRODUCTION

Modelling and optimising anaerobic digestion (AD) processes is critical for designing wastewater treatment and biogas plants, evaluating system performance, and assessing the feasibility of diverse substrates under varying conditions [8]. AD models are broadly categorized as mechanistic models, which rely on biological, physical, and chemical principles, or empirical machine learning models, which leverage observed process data to establish relationships between inputs and outputs [8]. Mechanistic models describe AD processes through differential equations that capture bacterial growth, inhibition, and physico-chemical interactions. These models range in complexity: simpler ones address single-step processes, intermediate models like AM2 [6] incorporate multiple microbial populations and interactions, and advanced models such as ADM1 [5] offer comprehensive system descriptions but demand extensive parameter estimation. The AM2 model, in particular, balances simplicity and accuracy, making it suitable for monitoring and controlling AD processes rather than detailed simulations [9]. Machine learning techniques such as k-nearest neighbors (KNN), support vector machines (SVM), random forests (RF), artificial neural networks (ANN), Dynamic Mode Decomposition (DMD), and the Koopman operator theory [8,3,12] have all been applied to model the complex, nonlinear interactions in AD processes. In this work, we use Gaussian Process (GP) a non-parametric, Bayesian approach to regression that models the underlying distribution of data as a continuous stochastic process [4]. A GP based approach is utilised because of its capacity to manage intricate and uncertain systems. While GPs have been applied in various fields, their use in predicting biogas production from AD has not yet been tested. This problem is critical given the need for reliable models to optimise biogas production from highly variable waste materials. The GP model is used to predict biogas production and other key performance indicators in a continuous anaerobic digester fed with hydrothermal carbonization (HTC) products [1]. The feedstock consists of hydrochar and HTC liquor derived from sewage sludge

and agro-industrial waste, which exhibit significant variability in composition and degradation profiles, complicating predictive modelling. The remainder of this paper is structured as follows. Section 2 outlines the experimental procedures and data collection process, followed by the development of a mechanistic model for anaerobic digestion and a data-driven modeling approach based on Multi-Task Gaussian Processes (MTGP). Section 3 explores the structure of the dataset, presents the outcomes of parameter estimation for the mechanistic model, and evaluates the performance of the MTGP framework. A comparative analysis is provided to assess the relative strengths and limitations of the mechanistic and MTGP approaches. The paper concludes with a summary of key findings and recommendations for future work.

METHODS

Experimental Setup and Data Generation

The dataset used in this study stems from a 164-day AD experiment with HTC biomass as the substrate, previously detailed by the authors in [9]. The experiments investigated the effects of HTC process conditions and operational parameters, such as dilution rate (D), influent soluble chemical oxygen demand ($SCOD_{in}$), organic loading rate (OLR), and pH, on AD performance metrics, including biogas yield, effluent SCOD, and volatile fatty acids (VFA) concentrations. Conducted in laboratory-scale reactors under controlled conditions (**Figure 1**), these experiments aimed to enhance the biodegradability of organic feedstocks for improved biogas production [1]. The mechanistic AM2 model [6] was applied to describe the AD system dynamics. The same parameter estimation and simulation procedures were applied from the original study [9], ensuring consistency and facilitating direct comparisons with the MTGP approach.

Mechanistic Model Development

In this study, the AM2 model developed within the framework of the Europe Research Project called AMOCO [6] is used due to its simplicity and accuracy in similar studies. The AM2 model represents AD in just two stages (Acidogenesis-Methanogenesis) and it is deduced from the mass balance law as in [9]:

$$\begin{aligned} \dot{S_1} &= D(S_{1in} - S_1) - k_1\mu_1(S_1)X_1 \\ \dot{X_1} &= (\mu_1(S_1) - k_{d1} - \alpha D)X_1 \\ \dot{S_2} &= D(S_{2in} - S_2) + k_2\mu_1(S_1)X_1 - k_3\mu_2(S_2)X_2 \\ \dot{X_2} &= (\mu_2(S_2) - k_{d2} - \alpha D)X_2 \end{aligned} \quad (1)$$

With

$$\mu_1(S_1) = \mu_{1max}\frac{S_1}{S_1+K_1}, \quad (2)$$

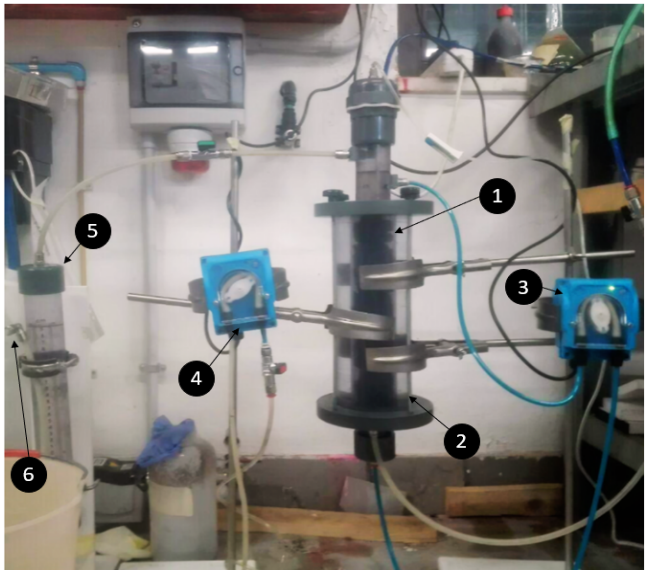

Figure 1. Laboratory picture of the anaerobic filter, in which: 1- Anaerobic filter, 2- Heating Jacket, 3- Recycle Pump, 4- Inlet Pump, 5- Biogas Measurement Device, 6- Outlet [1,9].

$$\mu_2(S_2) = \mu_{2max}\frac{S_2}{\frac{S_2^2}{K_i}+S_2+K_2}\left\{1 - \exp\left[-3\left(\frac{pH-pH_H}{pH_H-pH_L}\right)^2\right]\right\} \quad (3)$$

Where X_1 and X_2 represent the concentrations of acidogenic and methanogenic bacteria (g/L) respectively, while S_1 and S_2 denote the SCOD (g/L) and VFA (mmol/L) concentrations. k_i are the stoichiometric coefficients associated with the two reactions. $D = \frac{F}{V}$ and D is the dilution rate (F is the flow rate and V is the volume of the vessel), S_{1in} and S_{2in} are respectively the input concentrations of the substrates S_1 and S_2, and α is the fraction of the bacteria in the liquid phase. Death rates for X_1 and X_2 are k_{d1}, k_{d2}, respectively. The specific growth rate $\mu_1(S_1)$ and $\mu_2(S_2)$ are governed by Monod kinetics in (2) and Haldane kinetics in (3), with μ_{1max} and μ_{2max} as the maximum growth rates, K_1 and K_2 are the half-saturation constants, and K_i are the inhibition constant for S_2. Additionally, pH_L and pH_H define the lower and upper pH bounds, with inhibition effects on $\mu_2(S_2)$. The biogas flow rate (CH_4 plus CO_2) can be expressed as a function of the state variables given by:

$$Q_{biogas} = k_{gas}\mu_2(S_2)X_2 \quad (4)$$

Where k_{gas} is the yield for biogas production. To identify the model that best fits the experimental data, an appropriate criterion must be selected for optimising the model's parameter vector. Various cost functions are commonly used for parameter estimation in AD models, typically based on output-error criteria that quantify the discrepancy between model outputs and actual system outputs. [9]. The sum of least squares is a widely used and effective cost function in optimisation procedures,

especially when measurement error variances fluctuate over time.

$$J(\theta) = \min \sum_{t=1}^{N} \left(\frac{Y_{Measured}(t) - Y_{Model}(t,\theta)}{Y_{Measured}(t)} \right)^2 \quad (5)$$

Where J is the objective function to be minimised, $Y_{Measured}$ is the collected measurements vector, Y_{Model} is the model-predicted outputs vector with respect to model parameters θ to be determined and *N* is the number of measurements point. The measurements vector Y is defined by:

$$Y = \begin{bmatrix} S_1 & S_2 & Q_{biogas} \end{bmatrix}^T \quad (6)$$

The vector parameters θ is defined by:

$$\theta = \left[\mu_{1Max}, K_1, \mu_{2Max}, K_i, K_2, k_1, k_2, k_3, k_{gas} \right]^T \quad (7)$$

The other parameters α, k_{d1} and k_{d2} have been fixed with analogy to [9].

Multi-Task Gaussian Processes (MTGP)

Gaussian Process overview

A Gaussian Process (GP) is a non-parametric, Bayesian approach to regression that models the underlying distribution of data as a continuous stochastic process [4]. GPs are well-suited for complex, nonlinear systems, as they do not require explicit formulation of system dynamics. Instead, they operate by defining a prior distribution over functions that is updated as data is observed, making them a powerful tool in predicting outputs with uncertainty quantification. A GP is commonly viewed as a prior over functions $f: \mathbb{R}^P \to \mathbb{R}$ where P denotes the dimensionality of the input space. Consider a set of P-dimensional input points $\boldsymbol{X} \in \mathbb{R}^{P \times N}$ and corresponding scalar outputs $\boldsymbol{y} \in \mathbb{R}^N$. A GP is defined by a mean function, often assumed to be zero without loss of generality, and a kernel function $k: \mathbb{R}^P \times \mathbb{R}^P \to \mathbb{R}$, which measures the similarity between input points. The GP regression model with noisy observations is expressed as:

$$\boldsymbol{y_i} = f(\boldsymbol{x}_i) + \epsilon, \quad f \sim \mathcal{GP}\left(0, k(x_i, x_i')\right), \quad (8)$$

Where $\epsilon \sim \mathcal{N}(0, \sigma^2)$ represents Gaussian noise. Alternatively, this can be written as a multivariate normal distribution:

$$\boldsymbol{y} \sim \mathcal{N}(0, \boldsymbol{K}_{XX} + \sigma^2 \boldsymbol{I}_N), \quad (9)$$

where $\boldsymbol{K}_{XX} \in \mathbb{R}^{N \times N}$ is the kernel matrix formed by evaluating $k(x_i, x_j)$ for all pairs of input points, and $\boldsymbol{I}_N$ is the identity matrix. Given a new set of inputs $\boldsymbol{X}_* \in \mathbb{R}^{P \times M}$, the conditional distribution of the corresponding outputs $\mathbf{f}_* \in \mathbb{R}^M$ is:

$$\mathbf{f}_* | \, \boldsymbol{y}, \boldsymbol{X}, \boldsymbol{X}_* \sim \mathcal{N}(\mu, \Sigma), \quad (10)$$

Where:

$$\mu = \boldsymbol{K}_{\boldsymbol{X}_* \boldsymbol{X}} \boldsymbol{K}_{\boldsymbol{XX}}^{-1} \boldsymbol{y}, \quad (11)$$

$$\Sigma = \boldsymbol{K}_{\boldsymbol{X}_* \boldsymbol{X}_*} - \boldsymbol{K}_{\boldsymbol{X}_* \boldsymbol{X}} \boldsymbol{K}_{\boldsymbol{XX}}^{-1} \boldsymbol{K}_{\boldsymbol{X} \boldsymbol{X}_*}. \quad (12)$$

The presented traditional GPs are limited to producing a single scalar output, but in many cases, it is essential to explore the relationship between inputs and multiple outputs.

Multi-Output gaussian processes:

Standard GPs accommodate only a single scalar output. In practical applications, however, multiple outputs are often desired, such that $f: \mathbb{R}^P \to \mathbb{R}^Q$, where Q denotes the number of outputs. A naïve solution involves employing Q independent GPs, each modeling one output dimension [7]. However, this neglects correlations between outputs. To address this, advanced approaches like the Linear Model of Coregionalization (LMC) [10] have been developed. The LMC assumes L shared latent Gaussian processes $\{f_\ell\}_{\ell=1}^L$. The observed outputs for sample *i* are modeled as:

$$\boldsymbol{y_i} = \boldsymbol{W} \mathbf{f_i} + \boldsymbol{\epsilon}, \quad (13)$$

where $\mathbf{f_i} = [\mathrm{f_1(x_i)}, \ldots, \mathrm{f_L(x_i)}]^\top$, $\boldsymbol{W} \in \mathbb{R}^{\mathrm{Q} \times \mathrm{L}}$ is a matrix of loadings that maps latent functions to outputs, and $\boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{\sigma^2 I}_Q)$, Each latent function f_ℓ is drawn from a GP:

$$f_\ell \sim \mathcal{GP}(\boldsymbol{0}, \boldsymbol{K_\ell}) \quad (14)$$

where $\boldsymbol{K_\ell}$ is the kernel function for the $\boldsymbol{\ell}$-th latent GP. The covariance between outputs y_{iq} and $y_{jq'}$ is given by:

$$Cov(y_{iq}, y_{jq'}) = \sum_{\ell=1}^{L} k_\ell(\boldsymbol{x}_i, \boldsymbol{x}_j) w_{q\ell} w_{q'\ell}, \quad (15)$$

where $w_{q\ell}$ is the element of $\boldsymbol{W}$ at row q and column $\boldsymbol{\ell}$. The joint distribution of all outputs $\boldsymbol{Y}$ is multivariate normal:

$$vec(\boldsymbol{Y}) \sim \mathcal{N}(\boldsymbol{0}, \Sigma + \boldsymbol{\sigma^2 I}_{NQ}), \quad (16)$$

Where:

$$\Sigma = \sum_{\ell=1}^{L} \boldsymbol{K}_\ell \otimes \boldsymbol{w}_\ell \boldsymbol{w}_\ell^\top, \quad (17)$$

with $\otimes$ denoting the Kronecker product and $vec\,(\cdot)$ the vectorization operator. If all latent GPs share the same kernel function, the covariance simplifies to:

$$\Sigma = \boldsymbol{K} \otimes \boldsymbol{W} \boldsymbol{W}^\top, \quad (18)$$

This model captures output correlations through $\boldsymbol{W}$, allowing flexible multi-output modelling while preserving non-linearities from the latent GPs. For this study, the MTGP framework jointly models three key AD outputs: biogas production Q_{biogas}, SCOD, and VFA concentrations.

Each task is modelled by a shared latent function structure, leveraging the correlations between outputs to improve overall prediction accuracy. We adopt the LMC with a Radial Basis Function kernel for latent functions:

$$k(x, x') = \sum_{\ell=1}^{L} B_\ell \exp\left(-\frac{||x-x'||^2}{2l_\ell^2}\right), \quad (19)$$

where B_ℓ is a coregionalisation matrix for latent function ℓ, l_ℓ is the length scale, and L is the number of latent functions. The MTGP prior for task outputs $\mathbf{f} = [\mathbf{f}_1, \ldots, \mathbf{f}_D]$ follows:

$$\mathbf{f} \sim \mathcal{N}(0, \boldsymbol{K_f}), \quad (20)$$

where $\boldsymbol{K_f} = \sum_{\ell=1}^{L} \boldsymbol{B}_\ell \otimes \boldsymbol{K}_\ell(\boldsymbol{X}, \boldsymbol{X})$ capturing within-task and cross-task covariances. The MTGP model, trained over AD data across various conditions, maximises marginal likelihood using an Adam optimiser [11]. The likelihood is:

$$\log p(\boldsymbol{Y}|\boldsymbol{\theta}) = -\frac{1}{2}\boldsymbol{Y}^\top \boldsymbol{K_f^{-1}} \boldsymbol{Y} - \frac{1}{2}\log|\boldsymbol{K_f}| - \frac{nD}{2}\log(2\pi), \quad (21)$$

where $\boldsymbol{\theta}$ comprises hyperparameters. For new input $\boldsymbol{X}_*$ the predictive mean and variance are:

$$\boldsymbol{\mu}_* = \mathbf{K}(\mathbf{X}_*, \mathbf{X})\mathbf{K_f^{-1}}\mathbf{Y}, \quad (22)$$

$$\boldsymbol{\Sigma}_* = \boldsymbol{K}(\boldsymbol{X}_*, \boldsymbol{X}_*) - \boldsymbol{K}(\boldsymbol{X}_*, \boldsymbol{X})\boldsymbol{K_f^{-1}}\boldsymbol{K}(\boldsymbol{X}, \boldsymbol{X}_*). \quad (23)$$

These equations provide predictions along with uncertainty estimates, which are essential for assessing the reliability of all output's forecasts.

RESULTS AND DISSCUSION

Data Structure and Preprocessing

The dataset includes time-series input parameters (time, D, $SCOD_{in}$, OLR, and pH) and outputs (SCOD, VFA, and biogas production). Pre-processing steps included: i) Interpolation of missing or irregular data using cubic splines for consistent time scales; ii) Log transformation of outputs (with a small constant added) to stabilize variance and enhance model performance; and iii) Data splitting into training (one-third of the data) and testing subsets (half of the data) to ensure balanced coverage of operational variability for model development and validation. To assess the accuracy of the models, statistical metrics were calculated for each output, such as Root Mean Squared Error (RMSE) given by:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(Y_{Model,i} - Y_{Measuredi}\right)^2} \quad (24)$$

and the coefficient of determination (R^2) given by:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}\left(Y_{Measured,i} - Y_{Model,i}\right)^2}{\sum_{i=1}^{n}\left(Y_{Measured,i} - \overline{Y}_{Measured}\right)^2} \quad (25)$$

Where $\overline{Y}_{Measured}$: Mean of the observed values

Parameter Estimation for the AM2 Model

The AM2 model was employed to describe the dynamics of the AD process under investigation. Parameter estimation was conducted using the Pyomo optimisation framework with the IPOPT solver, offering an efficient and robust alternative to the MATLAB approach used in [9]. This procedure calibrated key kinetic and stoichiometric parameters based on a 164-day experimental dataset. Initial conditions and parameter guesses were derived from [9], and the optimisation problem was formulated as a nonlinear program. **Figure 2** compares model predictions for SCOD (S_1), VFA (S_2), and biogas production (Q_{biogas}) with experimental data, showing agreement. **Table 1** presents the estimated parameters, reflecting the kinetic and stoichiometric characteristics of the AD process. These parameters reflect the influence of HTC-treated substrates on microbial kinetics and reactor performance. The results confirm the utility of the AM2 model as a mechanistic tool for understanding and predicting the behavior of AD systems. The calibrated parameters provide valuable insights into substrate degradation and methane production dynamic, however there are clear areas of poor predictive performance.

Table 1: Estimated model parameter values

Parameter	Value	Unit
$\mu_{1_{max}}$	0.04	1/day
K_1	31.01	g/L
$\mu_{2_{max}}$	0.08	1/day
K_i	19.93	mmol/L
K_2	125.42	mmol/L
k_1	2374.50	--
k_2	2975.26	mmol/L
k_3	11558.51	mmol/L
k_{gas}	593	mmol/L

Multi-Task Gaussian Processes for Biogas Production Modeling

In this section, a data-driven approach was employed to predict AD outputs. The method leverages a MTGP framework, exploiting correlations among these multiple outputs to enhance predictive accuracy while providing uncertainty quantification. A dataset of N= 164 samples (where N corresponds to the total number of time points in the experiment) was compiled to include five operational parameters: time, dilution rate D, influent SCOD, OLR, and pH as inputs to the GP. These were stacked into a matrix $\mathbf{X} \in \mathbb{R}^{164\times5}$. Three outputs: SCOD, VFA, and biogas production, were similarly arranged into a matrix $\mathbf{Y} \in \mathbb{R}^{164\times3}$. The MTGP model leverages a variational inference strategy, enabling simultaneous

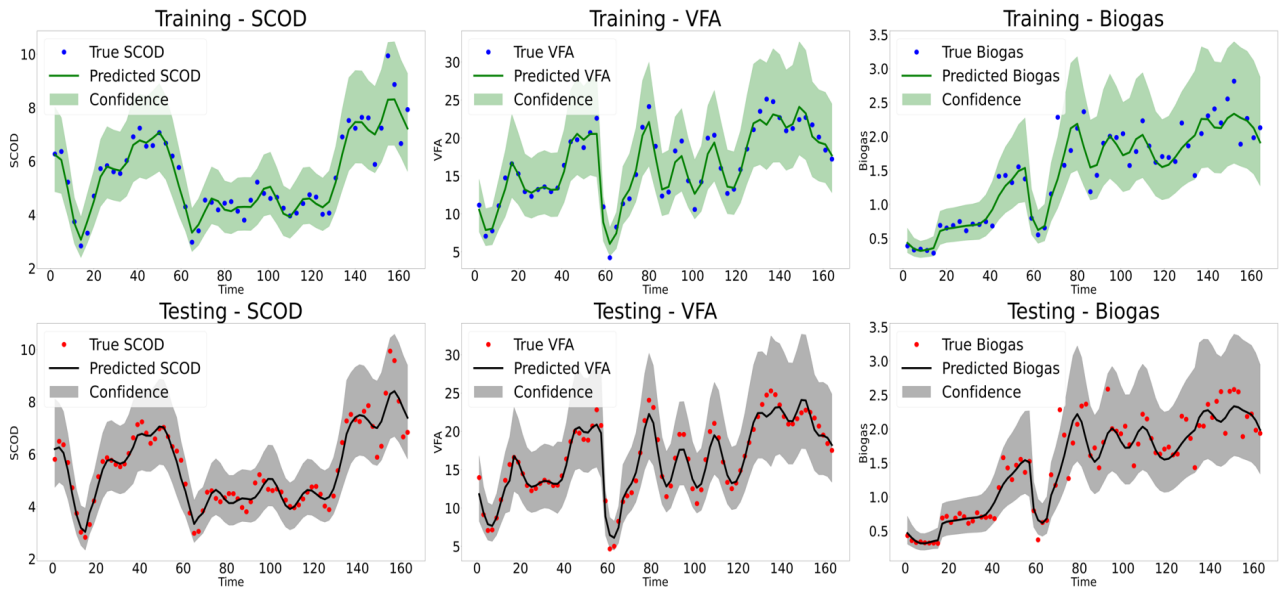

Figure 3: Comparison of MTGP model predictions with measured data for SCOD, VFA, and biogas production: training predictions and testing predictions, illustrating the model's performance in capturing AD outputs.

modelling of multiple outputs. Using the LMC with three latent functions, the model effectively shared information across tasks. With a training set of 55 data points, all served as inducing points, optimising computational efficiency for multi-output modelling. Confidence intervals provided insights into time points or operational regimes with greater uncertainty, crucial for real-world applications where factors like pH and substrate variability affect biogas yields. **Figure 3** illustrates the model's strong performance in tracking SCOD, VFA, and biogas production for both training and testing data, with confidence intervals conveying predictive accuracy and uncertainty. The MTGP framework demonstrated robust capabilities in capturing interdependencies among outputs, with inter-task learning enhancing predictive accuracy.

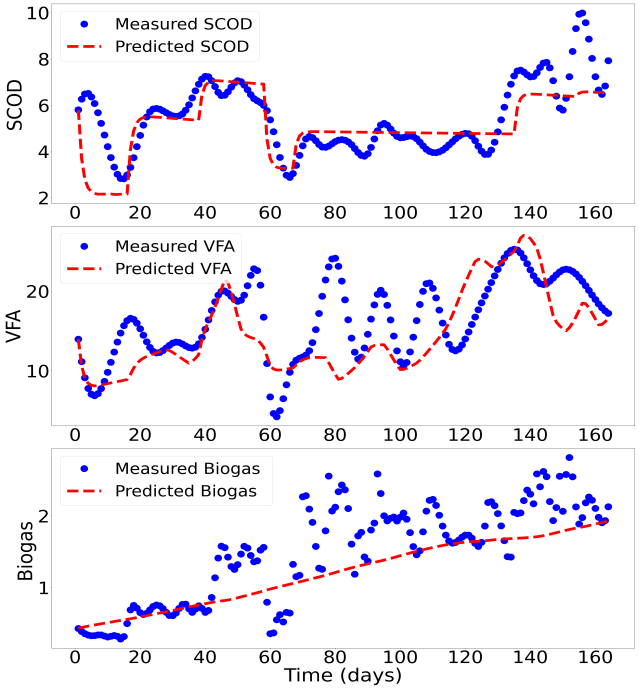

Figure 2. AM2 Model fit with experimental data using the set of optimal parameters obtained

Model Performance Comparison

The evaluation metrics presented in **Table 2** and **Table 3** highlight a performance difference between the AM2 mechanistic model and the MTGP model. For SCOD predictions, the MTGP model achieved a lower RMSE (0.32 g/L) and a higher R^2 value (0.91) compared to the AM2 model (RMSE: 1.37 g/L, R^2: 0.15) in this dataset.

Similarly, for VFA predictions, the MTGP model showed improved accuracy for the conditions tested, with an RMSE of 0.87 mmol/L and $R^2$of 0.94, appearing to outperform the AM2 model, which had an RMSE of 4.62 mmol/L and R^2 of 0.11. For biogas production, the MTGP model also showed better predictive performance with an RMSE of 0.15 L/day and R^2 of 0.88, as compared to the AM2 model's RMSE of 0.47 L/day and R^2 of 0.52. These results suggest that the MTGP model can leverage multi-task learning and inter-output correlations to potentially yield more accurate and reliable predictions across all key outputs in this study. The comparison between the AM2 mechanistic model and the MTGP model highlights complementary strengths in their approaches to modeling AD processes. While the MTGP model exhibits superior predictive accuracy, with significantly lower RMSE and higher R^2 values across all outputs (**Table 3**), the AM2 model's interpretability and biochemical grounding remain critical assets. The AM2 model captures the intricate biochemical and microbial dynamics of AD, which are essential for understanding the underlying system behavior. The AM2 model incorporates acidogenic/methanogenic biomass states, enhancing biological interpretability, but its reliance on unmeasured microbial groups and assumed kinetics (e.g., growth rates) introduces predictive uncertainty without experimental validation. In contrast, the MTGP avoids microbial complexity, simplifying calibration at the cost of mechanistic detail.

Table 2: The RMSE and R^2 for the AM2 model

Measurements	RMSE	R^2	Unit
SCOD(S_1)	1.37	0.15	g/L
VFA(S_2)	4.62	0.11	Mmol/L
Biogas (Q_{biogas})	0.47	0.52	L/day

Table 3: The RMSE and R^2 for the MTGP model

Measurements	RMSE	R^2	Unit
SCOD	0.32	0.91	g/L
VFA	0.87	0.94	Mmol/L
Biogas	0.15	0.88	L/day

CONCLUSION

This work demonstrates the application of Multi-Task Gaussian Processes as a powerful data-driven framework for modelling and predicting the performance of AD systems. By leveraging input-output correlations and employing the linear model of coregionalisation, the MTGP model demonstrated improved predictive accuracy compared to the AM2 mechanistic model. While MTGP showed strong predictive accuracy and adaptability in this context, the AM2 model provided essential interpretability and biochemical insights, underscoring the complementary strengths of these two approaches.

Future research should explore the integration of these two approaches into hybrid models that combine the interpretability of mechanistic frameworks with the predictive power of data-driven techniques.

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