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Analysis and Control of a Dynamic Model involving Methane Production in Anaerobic Digestion

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ABSTRACT

In this study, bifurcation analysis and multi-objective nonlinear model predictive control are performed on a dynamic model involving methane production in anaerobic digestion. Bifurcation analysis is a powerful mathematical tool used to deal with the nonlinear dynamics of any process. Several factors must be considered, and multiple objectives must be met simultaneously. The MATLAB program MATCONT was used to perform the bifurcation analysis. The MNLMPC calculations were performed using the optimization language PYOMO in conjunction with the state-of-the-art global optimization solvers IPOPT and BARON. The bifurcation analysis revealed branch and limit points. The MNLMC converged on the Utopia solution. The branch points (which cause multiple steady-state solutions from a singular point) are very beneficial because they enable the multiobjective nonlinear model predictive control calculations to converge to the Utopia point (the best possible solution) in the model.

Keywords: Bifurcation; Optimization; Control; Methane

Background

Methane is another valuable biofuel that has great potential as a renewable energy source. Methane is the chief constituent of biogas that is produced through the anaerobic process of decomposition of organic substances such as agricultural waste, food refuse, sewage sludge, and farm animal waste. Since biogenic methane can be generated whenever organic waste becomes available, it qualifies as a renewable energy source because it is created from recent organic matter, unlike fossil fuels.

One advantage of methane as a biofuel is its high energy content and its lower carbon dioxide emissions per unit of energy produced, making it more environmentally friendly than coal and oil. Another advantage of harnessing biogas as fuel is that it can trap methane that would otherwise escape into the atmosphere, where it would act as a greenhouse gas if not utilized.

Methane is directly usable for cooking, heating, and the production of electricity or can be upgraded to biomethane by cleaning the impurities and carbon dioxide from it. Biomethane has characteristics similar to conventional natural gas and can thus be injected into an established natural gas network and even used as vehicle fuel. However, issues such as infrastructure costs, methane leakage, and infrastructure use require careful attention and planning. Despite this, producing energy from methane as a biofuel is still an applicable approach to an environmentally-friendly energy system.

Anaerobic digestion proceeds through a series of tightly coupled microbial steps: The complex polymers, including carbohydrates, proteins, and lipids, are degraded in the initial hydrolysis stage into simpler soluble compounds, including sugars, amino acids, and long-chain fatty acids. This is often the rate-limiting step when particulate or lignocellulosic substrates need to be treated. Hydrolysis products are fermented during acidogenesis into volatile fatty acids, alcohols, hydrogen, carbon dioxide, and ammonia. These intermediates are transformed in the subsequent acetogenesis stage into acetate, hydrogen, and carbon dioxide, and these are the key substrates for methane production.

Methanogenesis is the final step in anaerobic digestion. This process is carried out by highly specialized Archaea, called methanogens, that thrive in strictly anaerobic environments. Methane production occurs via two mechanisms: acetoclastic methanogenesis, in which acetate is converted to methane and carbon dioxide, and hydrogenotrophic methanogenesis, in which methane is produced from the reduction of carbon dioxide by hydrogen. For instance, in digesters processing municipal or agricultural waste, acetoclastic methanogenesis accounts for the predominant methane production, whereas in hydrogenotrophic reactions, low hydrogen concentrations facilitate methane production.

The efficiency of methane production varies significantly with environmental factors and operating conditions. Temperature affects microbial growth, with most digesters being mesophilic or thermophilic. pH is another significant parameter; methanogens are extremely sensitive to acidity and are normally optimal at a pH around 7. Nutrient levels and HRT affect both bacterial growth and methane production. Substrates and disturbances, such as organic overloading or toxic compounds, may affect bacterial growth and trigger an accumulation of volatile fatty acids, leading to methanogenesis inhibition and reduced gas production.

In general, methane production through anaerobic digestion is a sustainable approach to waste-to-energy. The biogas produced from anaerobic digestion can be used for heating or power generation, or further processed into biomethane and injected into the natural gas distribution network. Additionally, methane emissions from waste could be mitigated through anaerobic digestion, as it offers benefits in reducing greenhouse gases.

Bernard, et al[1], on dynamical model development and parameter identification for anaerobic wastewater treatment processes. Álvarez-Ramírez, et al.[2] developed a J, feedback control design for an anaerobic digestion process. Steyer, et al.[3] conducted online measurements of COD, TOC, VFA, total and partial alkalinity in anaerobic digestion processes using infra-red spectrometry. Guay, et al.[4] performed adaptive extremum seeking control of continuous stirred tank bioreactors with unknown growth kinetics. Mailleret, et al.[5] developed nonlinear adaptive control procedures for bioreactors with unknown kinetics.

Méndez-Acosta, et al.[6] developed a robust feedforward/feedback control for an anaerobic digester. Shen, et al.[7] performed bifurcation and stability analysis of an anaerobic digestion model. Simeonov, et al.[8] researched identification and extremum seeking control of the anaerobic digestion of organic wastes. Méndez-Acosta, et al.[9] studied robust control of volatile fatty acids in anaerobic digestion processes. Hess, et al.[10] conducted studies on the design and risk management criteria for an unstable anaerobic wastewater treatment process.

Sbarciog, et al.[11] determined appropriate operation strategies for anaerobic digestion systems. Dimitrova[12] studied nonlinear adaptive stabilizing control of an anaerobic digestion model with unknown kinetics. Sbarciog, et al.[13] worked on the optimization of biogas production in anaerobic digestion systems. Serhani, et al.[14] performed dynamical studies and robustness for nonlinear wastewater treatment models. Benyahia, et al.[15] performed bifurcation and stability analysis of a two-step model for monitoring anaerobic digestion processes. Lara-Cisneros, et al.[16] worked on the dynamical behaviour of two-dimensional biological reactors. Flores-Estrella, et al.[17] studied H-infinity control strategies of anaerobic digester for winery industry wastewater treatment. Lara-Cisneros, et al.[18] developed an extremum seeking approach via variable-structure control for fed-batch bioreactors with uncertain growth rate. Lara-Cisneros, et al.[19] performed dynamic optimization calculations of methane production in anaerobic digestion via an extremum-seeking control approach. Methane production in anaerobic digestion is a highly complex and nonlinear process. This work aims to perform bifurcation analysis and multiobjective nonlinear control (MNLMPC) studies on a a dynamic model involving methane production in anaerobic digestion[19]. The paper is organized as follows. First, the model equations are presented, followed by a discussion of the numerical techniques involving bifurcation analysis and multiobjective nonlinear model predictive control (MNLMPC). The results are then presented, followed by the discussion and conclusions.

Model Equations

The organic substrate is s1, and x1 represents the acidogenic bacteria. The secondary substrate is s2. x2 is the methanogenic bacteria. s1f and s2f are the inlet concentrations of the primary and secondary organic substrates. The dilution rate is d. k1, k2, and k3 are the yield coefficients, and a represents the proportion of the bacterial population that is affected by the digester dilution. $\mu 1, \mu 2$ are the growth rate of the microorganisms. The dynamic equations are

$$
\begin{aligned}
mu1 &= \frac{\mu 1 max(s1)}{(ks1+s1)} \\
mu2 &= \frac{\mu 2 max(s2)}{\left(ks2+s2+\left(\frac{(s2)^2}{kl2}\right)\right)} \\
\frac{ds1}{dt} &= d(s1f-s1)-k1(\mu 1)x1 \\
\frac{dx1}{dt} &= \mu 1(x1)-a(d)x1 \\
\frac{ds2}{dt} &= d(s2f-s2)+k2(\mu 1)x1-k3(\mu 2)x2 \\
\frac{dx2}{dt} &= \mu 2(x2)-a(d)x2
\end{aligned}
\tag{1}
$$

The base parameters are k1=42.14;k2=116.5;k3=268; $\mu 1\max$ =0.05; $\mu 2\max$ =0.031; ks1=7.1;ks2=9.28;kl2=16;a=0.15; s1f=10;s2f=80;

More model details can be found in Lara-Cisneros, et al.[19].

Bifurcation analysis

Bifurcation analysis deals with multiple steady-states (caused by branch and limit points) and limit cycles, which are caused by Hopf bifurcation points. The MATLAB program MATCONT[20,21] is used to locate limit points, branch points, and Hopf bifurcation points. In ODE system

$$\frac{dx}{dt} = f(x,\alpha) \qquad (2)$$

$x \in R^n$ Let the bifurcation parameter be α . Since the gradient is orthogonal to the tangent vector,

The tangent plane is the n+1-dimensional vector w that satisfies

$$Aw = 0 \qquad (3)$$

Where A is

$$A = [\partial f/\partial x \quad | \partial f/\partial \alpha] \qquad (4)$$

And $\partial f/\partial x$ is the Jacobian matrix. For both limit and branch points, the Jacobian matrix $J = [\partial f/\partial x]$ must be singular.

For a limit point, there is only one tangent at the point of singularity. At this singular point, there is a single non-zero vector, y, where Jy=0. This vector is of dimension n. Since there is only one tangent the vector $y = (y_1, y_2, y_3, y_4, ... y_n)$ must align with $\hat{w} = (w_1, w_2, w_3, w_4, ... w_n)$. Since

$$J\hat{w} = Aw = 0 \qquad (5)$$

the n+1 th component of the tangent vector w_{n+1} = 0 at a limit point (LP).

For a branch point, there must exist two tangents at the singularity. Let the two tangents be z and w. This implies that

$$Az = 0$$
$$Aw = 0 \qquad (6)$$

Consider a vector v that is orthogonal to one of the tangents (say w). v can be expressed as a linear combination of z and w ($v = \alpha z + \beta w$). Since $Az = Aw = 0$; $Av = 0$ and since w and v are orthogonal, $w^T v = 0$. Hence $Bv = \begin{bmatrix} A \\ w^T \end{bmatrix} v = 0$ which implies that B is singular.

Hence, the matrix $B = \begin{bmatrix} A \\ w^T \end{bmatrix}$ is singular at a branch point.

When there is a Hopf bifurcation point the bialternate product,

$$\det(2 f_x(x,\alpha) @ Jn) = 0 \qquad (7)$$

where Jn is the n-square identity matrix. Hopf bifurcations cause limit cycles and should be eliminated because limit cycles make optimization and control tasks very difficult. More details can be found in Kuznetsov[22-24].

Multiobjective nonlinear model predictive control (MNLMPC)

The rigorous multiobjective nonlinear model predictive control (MNLMPC) method developed by Flores Tlacuahuaz, et al.[25] was used. Consider a problem where the variables $\sum_{t_{i=0}}^{t_i=t_f} q_j(t_i)$ have to be optimized together for a dynamic problem.

$$\frac{dx}{dt} = F(x,u) \qquad (8)$$

t_f being the final time value and u the control parameter.

The individual objective optimal control problem is solved by optimizing each of the variables $\sum_{t_{i=0}}^{t_i=t_f} q_j(t_i)$ The optimization of $\sum_{t_{i=0}}^{t_i=t_f} q_j(t_i)$ will lead to the values q_j^*. Then the multiobjective optimal control (MOOC) problem is solved. This will provide the value of u at each time step. The first obtained control value of u is implemented and this procedure is repeated until the implemented and the first obtained control values are the same or where ($\sum_{t_{i=0}}^{t_i=t_f} q_j(t_i) - q_j^* = 0$ for all j. Utopia point) is obtained.

$$\min (\sum_{j=1}^{n} (\sum_{t_{i=0}}^{t_i=t_f} q_j(t_i) - q_j^*))^2$$
$$subject\ to\ \frac{dx}{dt} = F(x,u); \qquad (9)$$

The optimization program PYOMO[26] is used. Here, the differential equations are converted to a Nonlinear Program (NLP) using the orthogonal collocation method. The NLP is solved using IPOPT[27] and confirmed as a global solution with BARON[28].

The steps of the algorithm are as follows

- Optimize $\sum_{t_{i=0}}^{t_i=t_f} q_j(t_i)$ and obtain q_j^*.
- Minimize $(\sum_{j=1}^{n} (\sum_{t_{i=0}}^{t_i=t_f} q_j(t_i) - q_j^*))^2$ and get the control values at various times.
- Implement the first obtained control values
- Repeat steps 1 to 3 until there is an insignificant difference between the implemented and the first obtained value of

the control variables or if the Utopia point is achieved. The Utopia point is when $\sum_{t_i=0}^{t_i=t_f} q_j(t_i) - q_j^* = 0$ for all j.

Sridhar[29] demonstrated that when the bifurcation analysis revealed the presence of limit and branch points the MNLMPC calculations to converge to the Utopia solution. This was done by imposing the singularity condition, caused by the presence of the limit or branch points on the co-state equation[30].

Results and Discussion

Theorem

If one of the functions in a dynamic system is separable into two distinct functions, a branch point singularity will occur in the system.

Proof

Consider a system of equations

$$\frac{dx}{dt} = f(x,\alpha) \quad (10)$$

$x \in R^n$. Defining the matrix A as

$$A = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} & \frac{\partial f_1}{\partial x_4} \cdots\cdots & \frac{\partial f_1}{\partial x_n} & \frac{\partial f_1}{\partial \alpha} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} & \frac{\partial f_2}{\partial x_4} \cdots\cdots & \frac{\partial f_2}{\partial x_n} & \frac{\partial f_2}{\partial \alpha} \\ \cdots & & & & & \\ \cdots & & & & & \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \frac{\partial f_n}{\partial x_3} & \frac{\partial f_n}{\partial x_4} \cdots\cdots & \frac{\partial f_n}{\partial x_n} & \frac{\partial f_n}{\partial \alpha} \end{bmatrix} \quad (11)$$

α is the bifurcation parameter. The matrix A can be written in a compact form as

$$A = [\frac{\partial f_p}{\partial x_q} . | \quad \frac{\partial f_p}{\partial \alpha}] \quad (12)$$

The tangent at any point x; $(z = [z_1, z_2, z_3, z_4, \ldots z_{n+1}])$ must satisfy

$$Az = 0 \quad (13)$$

The matrix $\{\frac{\partial f_p}{\partial x_q}\}$ must be singular at both limit and branch points. The n+1th component of the tangent vector z_{n+1} = 0 at a limit point (LP) and for a branch point (BP) the matrix $B = \begin{bmatrix} A \\ z^T \end{bmatrix}$ must be singular. Any tangent at a point y that is defined by $z = [z_1, z_2, z_3, z_4, \ldots z_{n+1}]$) must satisfy

$$Az = 0 \quad (14)$$

For a branch point, there must exist two tangents at the singularity. Let the two tangents be z and w. This implies that

$$Az = 0$$
$$Aw = 0 \quad (15)$$

Consider a vector v that is orthogonal to one of the tangents (say z). v can be expressed as a linear combination of z and w ($v = \alpha z + \beta w$). Since $Az = Aw = 0$; $Av = 0$ and since z and v are orthogonal, $z^T v = 0$. Hence $Bv = \begin{bmatrix} A \\ z^T \end{bmatrix} v = 0$ which implies that B is singular where $B = \begin{bmatrix} A \\ z^T \end{bmatrix}$

Let any of the functions f_i are separable into 2 functions ϕ_1, ϕ_2 as

$$f_i = \phi_1 \phi_2$$

At steady-state $f_i(x,\alpha) = 0$ and this will imply that either $\phi_1 = 0$ or $\phi_2 = 0$ or both ϕ_1 and ϕ_2 must be 0. This implies that two branches $\phi_1 = 0$ and $\phi_2 = 0$ will meet at a point where both ϕ_1 and ϕ_2 are 0.

At this point, the matrix B will be singular as a row in this matrix would be

$$[\frac{\partial f_i}{\partial x_k} | \frac{\partial f_i}{\partial \alpha}]$$

However,

$$[\frac{\partial f_i}{\partial x_k} = \phi_1(=0)\frac{\partial \phi_2}{\partial x_k} + \phi_2(=0)\frac{\partial \phi_1}{\partial x_k} = 0(\forall k = 1.,,n)$$
$$\frac{\partial f_i}{\partial \alpha} = \phi_1(=0)\frac{\partial \phi_2}{\partial \alpha} + \phi_2(=0)\frac{\partial \phi_1}{\partial \alpha}] = 0$$

This implies that every element in the row $[\frac{\partial f_i}{\partial x_k} | \frac{\partial f_i}{\partial \alpha}]$ would be 0, and hence the matrix B would be singular. The singularity in B implies that there exists a branch point.

When d was the bifurcation parameter 2 branch points were found at (s1, x1, s2, x2, d) values of (10, 0, 80, 0, 0.033791) and (10, 0, 80, 0, 0.194932) **(Figure 1a)**.

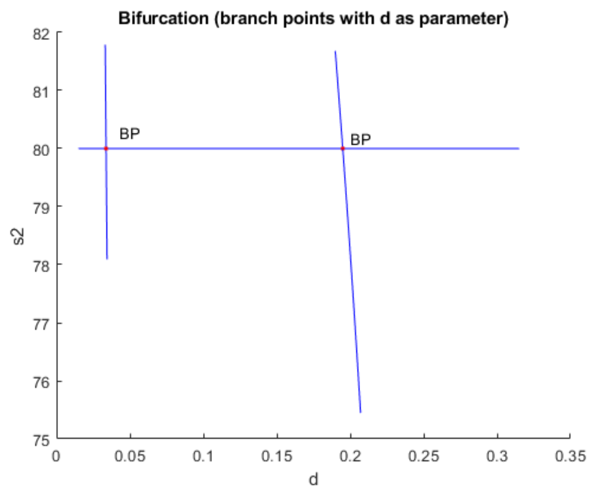

Figure 1a: Branch points with d as bifurcation parameter.

For the first branch point, the two distinct functions can be obtained from the fourth ODE in the model

$$\frac{dx2}{dt} = \mu 2(x2) - a(d)x2$$
$$\mu 2 = \frac{\mu 2max(s2)}{\left(ks2 + s2 + \left(\frac{(s2)^2}{kl2}\right)\right)} \quad (16)$$

The two distinct equations are

$$x2 = 0$$
$$\frac{\mu 2max(s2)}{\left(ks2 + s2 + \left(\frac{(s2)^2}{kl2}\right)\right)} - a(d) = 0 \quad (17)$$

With x2=0; d=0.033791; s2= 80; ks2=9.28; kl2=16; $\mu 2\max$ =0.031; a=0.15; both distinct equations are satisfied, validating the theorem.

For the second branch point, the two distinct functions can be obtained from the second ODE in the model

$$\frac{dx1}{dt} = \mu 1(x1) - a(d)x1$$
$$\mu 1 = \frac{\mu 1max(s1)}{(ks1 + s1)} \quad (18)$$

The two distinct equations are

$$x1 = 0$$
$$\frac{\mu 1max(s1)}{(ks1 + s1)} - a(d) = 0 \quad (19)$$

With x1=0; d=0.194932; s1= 10, ks1=7.1, $\mu 1\max$ =0.05, a=0.15; both distinct equations are satisfied, validating the theorem.

A limit point was located at (2.313002, 1.216105, 12.185335, 2.215575, 0.081908) **(Figure 1b)**.

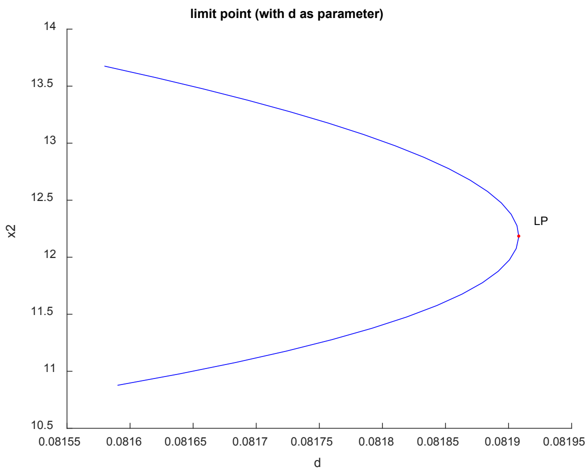

Figure 1b: Limit point with d as bifurcation parameter.

For the MNLMPC, d is the control parameter, and $\sum_{t_{i=0}}^{t_i=t_f}(\mu 1x1(t_i)), \sum_{t_{i=0}}^{t_i=t_f}(\mu 2x2(t_i))$ are maximized and individually, and led to values of 0.78162 and 1.059. The overall optimal control problem will involve the minimization of $(\sum_{t_{i=0}}^{t_i=t_f}(\mu 1x1(t_i)) - 0.78162)^2 + (\sum_{t_{i=0}}^{t_i=t_f}(\mu 2x2(t_i)) - 1.059)^2$ was minimized subject to the equations governing the model. This led to a value of zero (the Utopia point). The MNLMPC values of the control variable d is 0.2. The MNLMPC profiles are shown in **(Figures 2a-2e)**. The presence of the branch and limit points causes the MNLMPC calculations to attain the Utopia solution, validating the analysis of Sridhar[29].

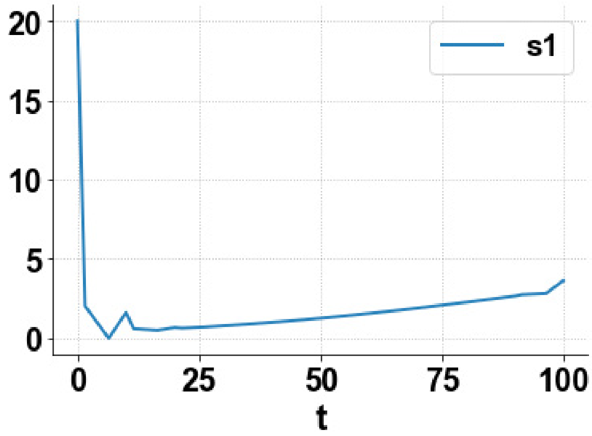

Figure 2a: MNLMPC s1 vs t.

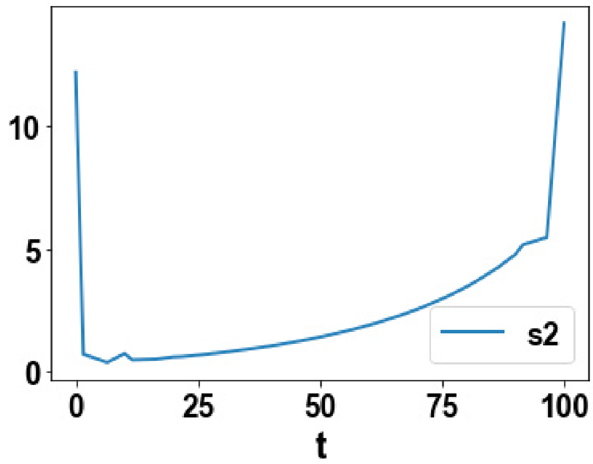

Figure 2b: MNLMPC s2 vs t.

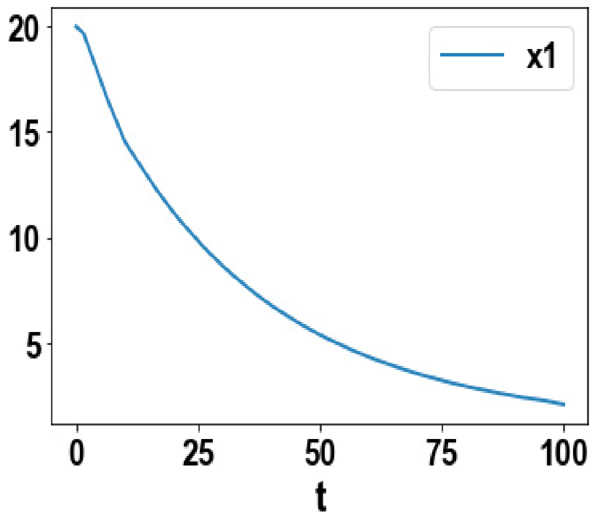

Figure 2c: MNLMPC x1 vs t.

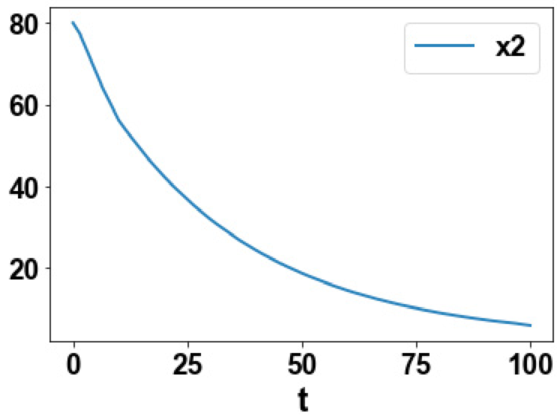

Figure 2d: MNLMPC x2 vs t.

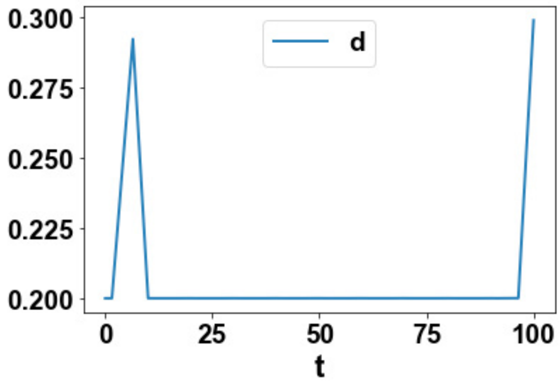

Figure 2e: MNLMPC d vs t.

Conclusions

Bifurcation analysis and multiobjective nonlinear control (MNLMPC) studies are conducted on a dynamic model involving methane production in anaerobic digestion. The bifurcation analysis revealed branch and limit points. The branch and limit points (which cause multiple steady-state solutions from a singular point) are very beneficial because they enable the Multiobjective nonlinear model predictive control calculations to converge to the Utopia point (the best possible solution) in the model. A combination of bifurcation analysis and Multiobjective Nonlinear Model Predictive Control (MNLMPC) for a dynamic model involving methane production in anaerobic digestion is the main contribution of this paper.

Data Availability Statement

All data used is presented in the paper.

Conflict of Interest

The author, Dr. Lakshmi N Sridhar has no conflict of interest.

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