

Analysis and Control of the Activated Sludge Model (ASM1)

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Abstract

Water pollution poses a considerable threat to public health, and it is important to understand water pollution transmission dynamics. This paper presents a mathematical framework involving bifurcation analysis and multiobjective nonlinear model predictive control (MNLMP) for two models involving water pollution. Bifurcation analysis is a powerful mathematical tool used to address the nonlinear dynamics of any process. The MATLAB program MATCONT was utilized to conduct the bifurcation analysis of the water pollution models. Several factors must be taken into account, and multiple objectives must be achieved simultaneously. The MNLMP calculations for the water pollution models were performed using the optimization language PYOMO in conjunction with the advanced global optimization solvers IPOPT and BARON. The bifurcation analysis revealed the presence of branch points in the two models. These branch points are advantageous as they allow the multiobjective nonlinear model predictive control calculations to converge to the Utopia point, which represents the most beneficial solution. The combination of bifurcation analysis and multiobjective nonlinear model predictive control for models involving water pollution is the main contribution of this paper.

Key words: water pollution; bifurcation; optimization; control

Introduction

To minimize effluent contamination concentrations, wastewater treatment plants use the activated sludge process. This process should be conducted efficiently, keeping all unnecessary expenses to a minimum. To achieve this goal, there has been a lot of modelling work to understand the various chemical reactions involved in this process. Henze et al (1987) [1] developed a general model for single-sludge wastewater treatment systems. Henze et al (1995) [2] extended and improved this earlier model.

Henze (1999) [3] performed modelling work on the aerobic wastewater treatment processes taking into account environmental impacts. Gujer et al (1995) [4] further improved upon the models of Henze. Fikar et al (2005) [5] developed strategies to ensure the optimal operation of alternating activated sludge processes. Yoon et al (2005) [6], Critical operational parameters for zero sludge production in biological wastewater treatment processes combined with sludge disintegration. Nelson et al (2009) [7] used continuation methods to determine the steady-state behaviour of the activated sludge model (ASM1).

The activated sludge models are highly nonlinear, and many factors must be taken into account to ensure that the process is conducted most efficiently. In this article, a combination of bifurcation analysis and multiobjective nonlinear model predictive control (MNLMP) for the activated sludge model (ASM1) (Nelson et al, 2009) [7] is performed. The bifurcation analysis reveals the presence of branch points, which are very beneficial because they enable the MNLMP calculations to converge to the Utopia point, which is the best possible solution.

This paper is organized as follows. First, the ASM1 model equations (Nelson et al, 2009) [7] are presented. The numerical procedures (bifurcation analysis and multiobjective nonlinear model predictive control (MNLMP)) are then described. This is followed by the results and discussion and conclusions.

ASM1 model equations

$$\begin{aligned} \frac{dS_s}{dt} &= d(S_{s,in} - S_s) - \frac{\mu_{MAX,H}}{Y_H} M_2 (M_{8h} + I_8 M_9 \eta_g) X_{BH} + k_h k_{sd} (M_{8h} + I_8 M_9 \eta_g) X_{BH} \\ \frac{dX_s}{dt} &= d(X_{s,in} - X_s) + d(b-1)X_s + (1-f_p)(b_H X_{BA} + b_A X_{BA}) - k_h k_{sd} (M_{8h} + I_8 M_9 \eta_g) X_{BH} \\ \frac{dX_{BH}}{dt} &= d(X_{BH,in} - X_{BH}) + d(b-1)X_{BH} + \mu_{MAX,H} M_2 (M_{8h} + I_8 M_9 \eta_g) X_{BH} - b_H X_{BH} \\ \frac{dX_{BA}}{dt} &= d(X_{BA,in} - X_{BA}) + d(b-1)X_{BA} + \mu_{MAX,A} M_{10} M_{8A} X_{BA} - b_H X_{BA} \\ \frac{dS_O}{dt} &= d(S_{O,in} - S_O) - \frac{(1-Y_H)}{Y_H} \mu_{MAX,H} M_2 M_{8h} X_{BH} - \frac{(4.57-Y_A)}{Y_A} \mu_{MAX,A} M_{10} M_{8A} X_{BA} \\ \frac{dS_{NO}}{dt} &= d(S_{NO,in} - S_{NO}) - \frac{(1-Y_H)}{2.86 Y_H} \mu_{MAX,H} M_2 I_8 M_9 \eta_g X_{BH} + \frac{1}{Y_A} \mu_{MAX,A} M_{10} M_{8A} X_{BA} \\ \frac{dS_{NH}}{dt} &= d(S_{NH,in} - S_{NH}) - i_{XB} \mu_{MAX,H} M_2 (M_{8h} + I_8 M_9 \eta_g) X_{BH} - (i_{XB} + \frac{1}{Y_A}) \mu_{MAX,A} M_{10} M_{8A} X_{BA} + K_A S_{ND} X_{BH} \\ \frac{dS_{ND}}{dt} &= d(S_{ND,in} - S_{ND}) - K_A S_{ND} X_{BH} + K_H K_{SAT} (M_{8h} + I_8 M_9 \eta_g) X_{BH} \frac{X_{ND}}{X_S} \\ \frac{dX_{ND}}{dt} &= d(X_{ND,in} - X_{ND}) + d(b-1)X_{ND} + (i_{XB} - f_p i_{XP})(b_H X_{BA} + b_A X_{BA}) - K_H K_{SAT} (M_{8h} + I_8 M_9 \eta_g) X_{BH} \frac{X_{ND}}{X_S} \end{aligned} \quad (1)$$

Where.,

$$M_2 = \frac{S_s}{(K_s + S_s)}; M_{8a} = \frac{S_o}{(K_{oa} + S_o)}; M_{8b} = \frac{S_o}{(K_{ob} + S_o)}; M_9 = \frac{S_{No}}{(K_{No} + S_{No})};$$

$$M_{10} = \frac{S_{NH}}{(K_{NH} + S_{NH})}; I_8 = \frac{K_{oh}}{(K_{oh} + S_o)}; K_{sat} = \frac{X_s}{((K_s(X_{bh}) + X_s))};$$

The parameter values are

$$K_{LA} = 4; K_{NH} = 1; K_{NO} = 0.5; K_{OA} = 0.4; K_{OH} = 0.2; K_s = 20; K_x = 0.03; S_{ND,in} = 9; S_{NH,in} = 15;$$

$$S_{NO,in} = 1; S_{Omax} = 10; S_{s,in} = 200; X_{BA,in} = 0; X_{BH,in} = 0; S_{o,in} = 2;$$

$$X_{ND,in} = 0; X_{p,in} = 0; X_{s,in} = 100; Y_A = 0.24; Y_H = 0.67; ba = 0.05; bh = 0.22;$$

$$fp = 0.08; I_{ab} = 0.086; I_{sp} = 0.06; K_a = 0.081; K_h = 3; \eta_g = 0.8; \eta_h = 0.4;$$

The variables $S_s, X_s, X_{BH}, X_{BA}, S_o, S_{NO}, S_{NH}, S_{ND}, X_{ND}$ represent the concentrations of readily biodegradable soluble substrate, slowly biodegradable particulate substrate, active heterotrophic particulate mass, active autotrophic particulate mass, soluble oxygen, soluble nitrate and nitrite nitrogen, soluble ammonium nitrogen, soluble biodegradable organic material, and particulate biodegradable organic nitrogen.

Bifurcation analysis

The MATLAB software MATCONT is used to perform the bifurcation calculations. Bifurcation analysis deals with multiple steady-states and limit cycles. Multiple steady states occur because of the existence of branch and limit points. Hopf bifurcation points cause limit cycles. A commonly used MATLAB program that locates limit points, branch points, and Hopf bifurcation points is MATCONT (Dhooge Govearts, and Kuznetsov, 2003[8]; Dhooge Govearts, Kuznetsov, Mestrom and Riet, 2004[9]). This program detects Limit points (LP), branch points (BP), and Hopf bifurcation points (H) for an ODE system

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

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

The tangent plane at any point $W = [w_1, w_2, w_3, w_4, \dots, w_{n+1}]$ must satisfy

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

Where A is

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

where $\partial f / \partial x$ is the Jacobian matrix. For both limit and branch points, the matrix $[\partial f / \partial x]$ must be singular. The $n+1$ th component of the tangent vector $w_{n+1} = 0$ for a limit point (LP) and for a branch point (BP)

the matrix $\begin{bmatrix} A \\ w^T \end{bmatrix}$ must be singular. At a Hopf bifurcation point,

$$\det(2f_x(x, \alpha) @ I_n) = 0 \quad (5)$$

@ Indicates the bialternate product while I_n 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 (1998 [10]; 2009[11]) and Govaerts [2000] [12]

Multiobjective Nonlinear Model Predictive Control (MNLMPCC)

Flores Tlacuahuaz et al (2012) [13] developed a multiobjective nonlinear model predictive control (MNLMPCC) method that is rigorous and does not involve weighting functions or additional constraints. This procedure is used

for performing the MNLMPCC calculations Here $\sum_{t_i=0}^{t_i=t_f} q_j(t_i)$ ($j=1, 2, n$)

represents the variables that need to be minimized/maximized simultaneously for a problem involving a set of ODE

$$\frac{dx}{dt} = F(x, u) \quad (6)$$

t_f being the final time value, and n the total number of objective variables and u the control parameter. This MNLMPCC procedure first solves the single objective optimal control problem independently optimizing each of the

variables $\sum_{t_i=0}^{t_i=t_f} q_j(t_i)$ individually. The minimization/maximization of

$\sum_{t_i=0}^{t_i=t_f} q_j(t_i)$ will lead to the values q_j^* . Then the optimization problem

that will be solved is

$$\min(\sum_{j=1}^n (\sum_{t_i=0}^{t_i=t_f} q_j(t_i) - q_j^*))^2 \quad (7)$$

$$\text{subject to } \frac{dx}{dt} = F(x, u);$$

This will provide the values of u at various times. The first obtained control value of u is implemented and the rest are discarded. This procedure is repeated until the implemented and the first obtained control values are the

same or if the Utopia point where $(\sum_{t_i=0}^{t_i=t_f} q_j(t_i) = q_j^*)$ for all j) is

obtained.

Pyomo (Hart et al, 2017) [14] is used for these calculations. Here, the differential equations are converted to a Nonlinear Program (NLP) using the orthogonal collocation method. The NLP is solved using IPOPT (Wächter And Biegler, 2006) [15] and confirmed as a global solution with BARON (Tawarmalani, M. and N. V. Sahinidis 2005) [16].

The steps of the algorithm are as follows

1. Optimize $\sum_{t_i=0}^{t_i=t_f} q_j(t_i)$ and obtain q_j^* at various time intervals t_i . The subscript i is the index for each time step.
2. 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 for various times.
3. Implement the first obtained control values
4. 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

$$\text{Utopia point is when } \sum_{t_i=0}^{t_i=t_f} q_j(t_i) = q_j^* \text{ for all } j.$$

Sridhar (2024) [17] proved that the MNLMPC calculations to converge to the Utopia solution when the bifurcation analysis revealed the presence of limit and branch points. This was done by imposing the singularity condition

on the co-state equation (Upreti, 2013) [18]. If the minimization of q_1 lead to the value q_1^* and the minimization of q_2 lead to the value q_2^* . The MNLMPC calculations will minimize the function $(q_1 - q_1^*)^2 + (q_2 - q_2^*)^2$. The multiobjective optimal control problem is

$$\min (q_1 - q_1^*)^2 + (q_2 - q_2^*)^2 \quad \text{subject to} \quad \frac{dx}{dt} = F(x, u) \quad (8)$$

Differentiating the objective function results in

$$\frac{d}{dx_i} ((q_1 - q_1^*)^2 + (q_2 - q_2^*)^2) = 2(q_1 - q_1^*) \frac{d}{dx_i} (q_1 - q_1^*) + 2(q_2 - q_2^*) \frac{d}{dx_i} (q_2 - q_2^*) \quad (9)$$

The Utopia point requires that both $(q_1 - q_1^*)$ and $(q_2 - q_2^*)$ are zero.

Hence

$$\frac{d}{dx_i} ((q_1 - q_1^*)^2 + (q_2 - q_2^*)^2) = 0 \quad (10)$$

the optimal control co-state equation (Upreti; 2013) is

$$\frac{d}{dt}(\lambda_i) = -\frac{d}{dx_i} ((q_1 - q_1^*)^2 + (q_2 - q_2^*)^2) - f_x \lambda_i; \quad \lambda_i(t_f) = 0 \quad (11)$$

λ_i is the Lagrangian multiplier. t_f is the final time. The first term in this equation is 0 and hence

$$\frac{d}{dt}(\lambda_i) = -f_x \lambda_i; \quad \lambda_i(t_f) = 0 \quad (12)$$

At a limit or a branch point, for the set of ODE $\frac{dx}{dt} = f(x, u)$ f_x is

singular. Hence there are two different vectors-values for $[\lambda_i]$ where $\frac{d}{dt}(\lambda_i) > 0$ and $\frac{d}{dt}(\lambda_i) < 0$. In between there is a vector $[\lambda_i]$ where $\frac{d}{dt}(\lambda_i) = 0$. This coupled with the boundary condition $\lambda_i(t_f) = 0$ will

lead to $[\lambda_i] = 0$. This makes the problem an unconstrained optimization problem, and the only solution is the Utopia solution.

Results and Discussion

The bifurcation analysis on the ASM1 model revealed the existence of two branch points at

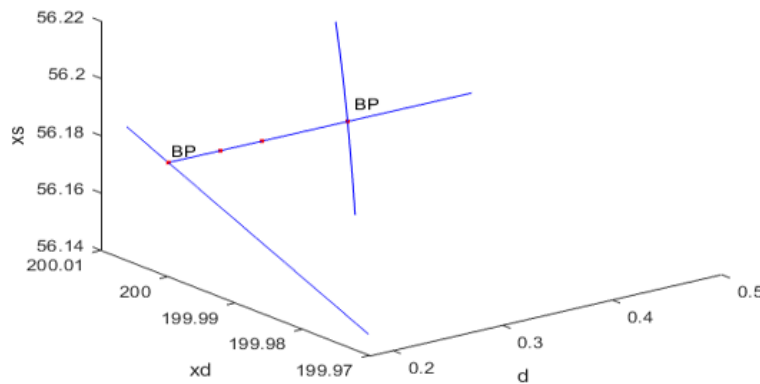


Figure 1: Branch points for ASM1 model

$(S_s, X_s, X_{BH}, X_{BA}, S_o, S_{NO}, S_{NH}, S_{ND}, X_{ND}, d)$ values of (200, 56.179, 0, 0.9.65, 1, 15, 9, 0, 0.179) and (200.000000 56.179, 0, 0.9.36, 1, 15, 9, 0.0.343). These branch points are indicated in Fig. 1. The presence of the branch points is beneficial because they allow the MNLMPC calculations to attain the Utopia solution for several objective functions.

Three MNLMPC calculations were performed. In the first case, the particulate variables (active heterotrophic particulate mass, active autotrophic particulate mass, and particulate biodegradable organic nitrogen)

were minimized. In this case, $\sum_{t_i=0}^{t_i=t_f} X_{BH}(t_i)$, $\sum_{t_i=0}^{t_i=t_f} X_{BA}(t_i)$, $\sum_{t_i=0}^{t_i=t_f} X_{ND}(t_i)$

was minimized individually and each of them led to a value of 0. The

overall optimal control problem will involve the minimization of $(\sum_{t_i=0}^{t_i=t_f} X_{BH}(t_i))^2 + (\sum_{t_i=0}^{t_i=t_f} X_{BA}(t_i))^2 + (\sum_{t_i=0}^{t_i=t_f} X_{ND}(t_i))^2$ was minimized subject to the equations governing the model. This led to a value of zero (the Utopia solution).

The various concentration profiles for this MNLMPC calculation are shown in Figures. 2a-2d.

The obtained control profile of s exhibited noise (Figure. 2e). This was remedied using the Savitzky-Golay Filter. The smoothed-out version of this profile is shown in Figure.2f.

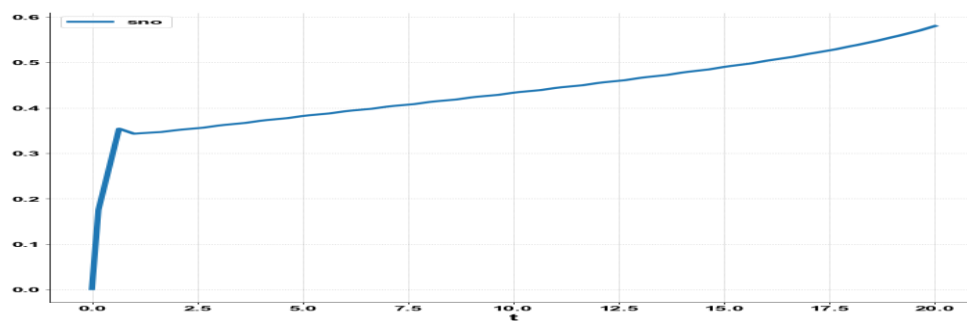


Figure 2a: SNO profile MNLMPc particulate concentration minimization

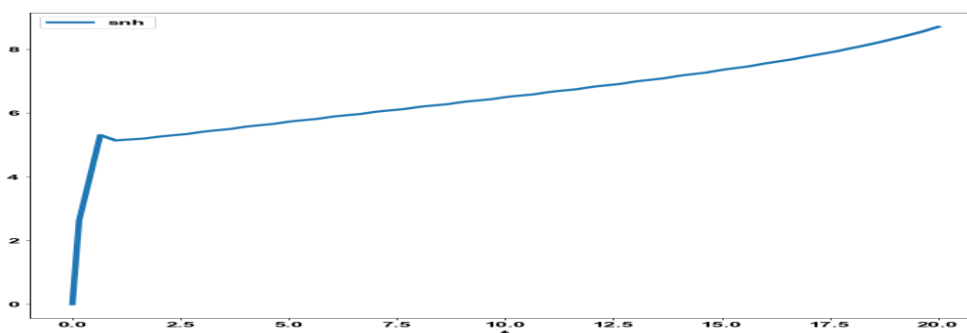


Figure 2b: SNH profile MNLMPc particulate concentration minimization

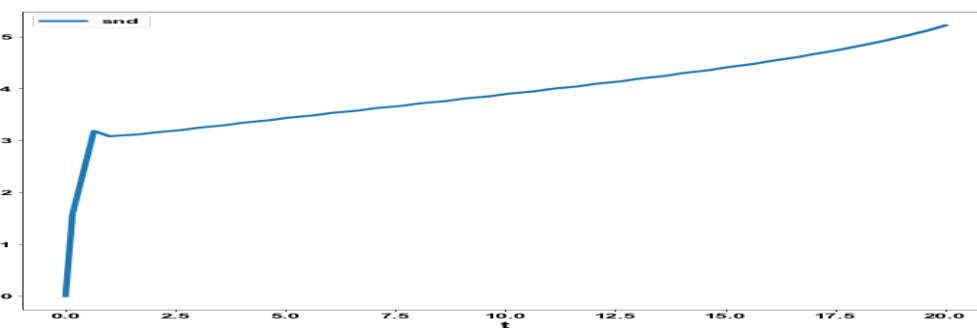


Figure 2c: SNO profile MNLMPc particulate concentration minimization

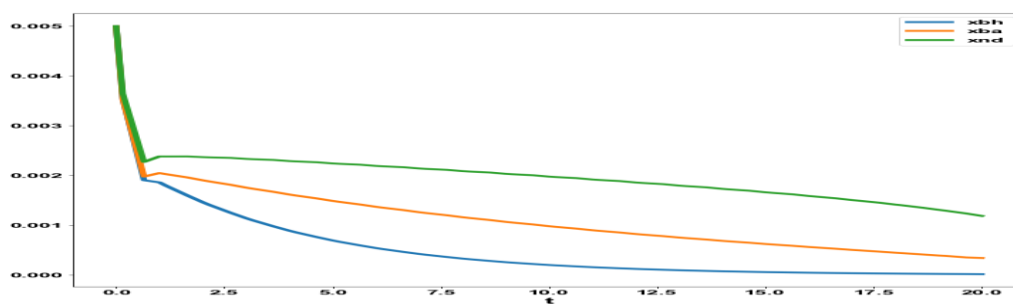


Figure 2d: XBH, XBA, XND profile MNLMPc particulate concentration minimization

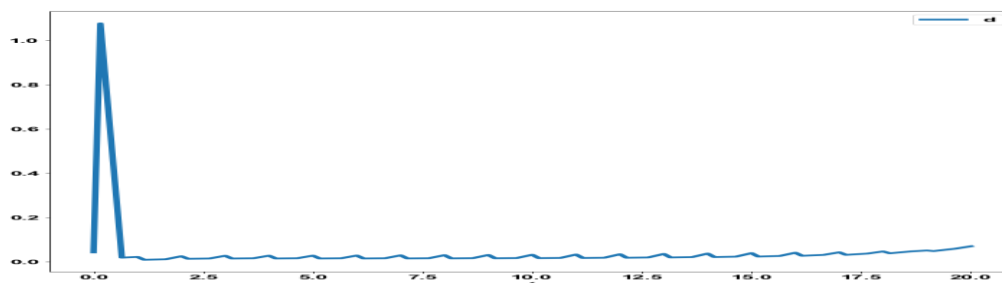


Figure 2e: dilution rate MNLMPc particulate concentration minimization

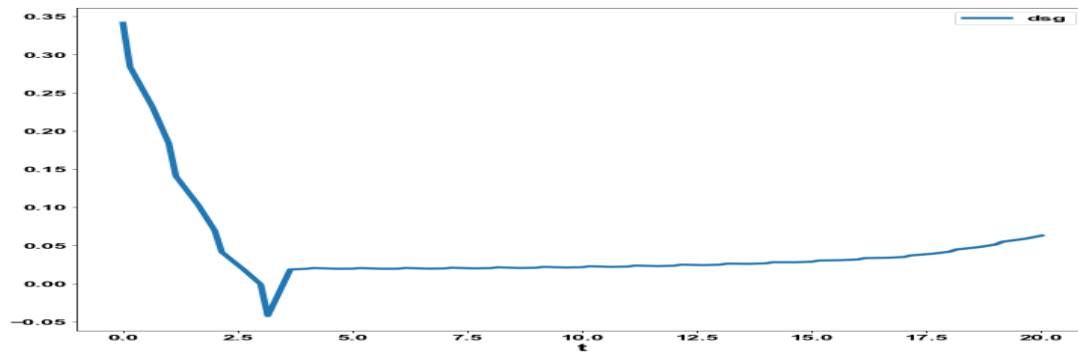


Figure 2f: dilution rate (with Savitzky Golay filter) MNLMPc particulate concentration minimization

In the second case, the variables representing the soluble materials (soluble nitrate and nitrite nitrogen, soluble ammonium nitrogen, and soluble biodegradable organic material) were minimized. In this case,

$\sum_{t_i=0}^{t_i=t_f} S_{NO}(t_i)$, $\sum_{t_i=0}^{t_i=t_f} S_{NH}(t_i)$, $\sum_{t_i=0}^{t_i=t_f} S_{ND}(t_i)$ was minimized individually,

leading to values of 0.4121, 4.722, and 0.019971. The overall optimal control problem will involve the minimization of

$$\left(\sum_{t_i=0}^{t_i=t_f} S_{NO}(t_i) - 0.4121 \right)^2 + \left(\sum_{t_i=0}^{t_i=t_f} S_{NH}(t_i) - 4.722 \right)^2 + \left(\sum_{t_i=0}^{t_i=t_f} S_{ND}(t_i) - 0.019971 \right)^2$$

was minimized subject to the equations governing the model. This led to a value of zero (the Utopia solution).

The various concentration profiles for this MNLMPc calculation are shown in Figs. 3a-3d.

The obtained control profile of s exhibited noise (Fig. 3e). This was remedied using the Savitzky-Golay Filter. The smoothed-out version of this profile is shown in Fig.3f.

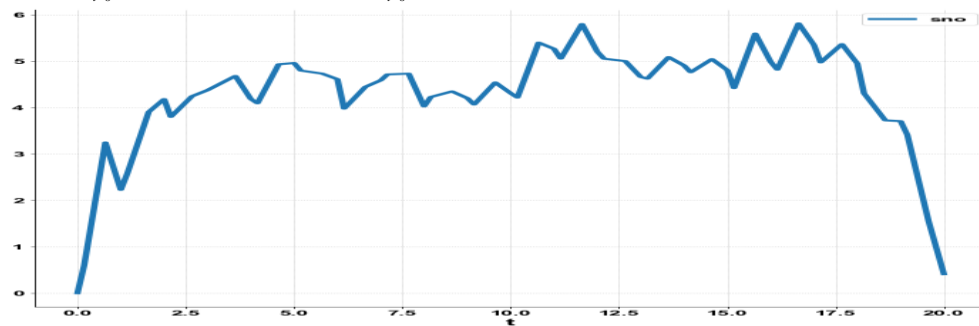


Figure 3a: SNO profile MNLMPc soluble material concentration minimization

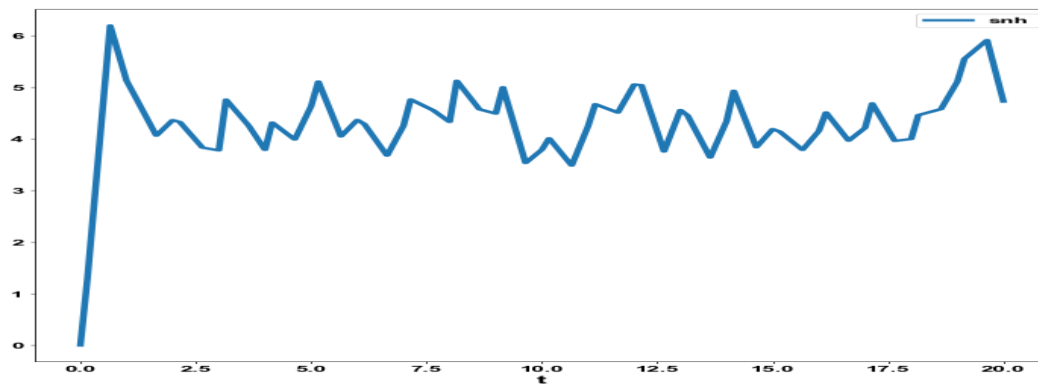


Figure 3b: SNH profile MNLMPc soluble material concentration minimization

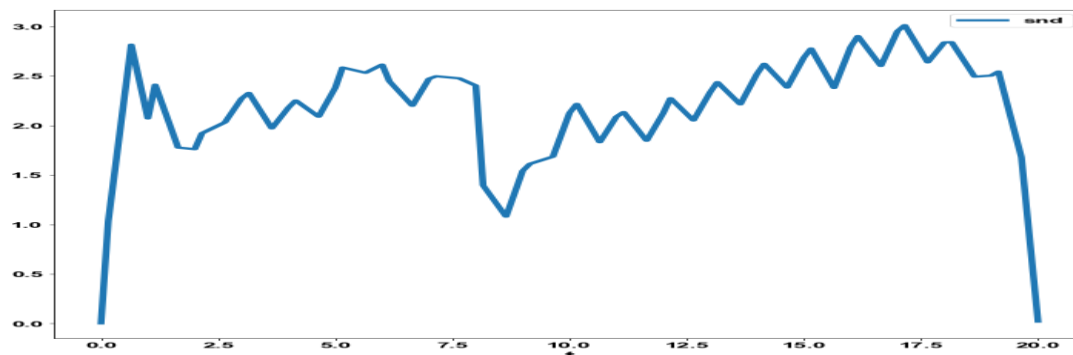


Figure 3c: SND profile MNLMPc soluble material concentration minimization

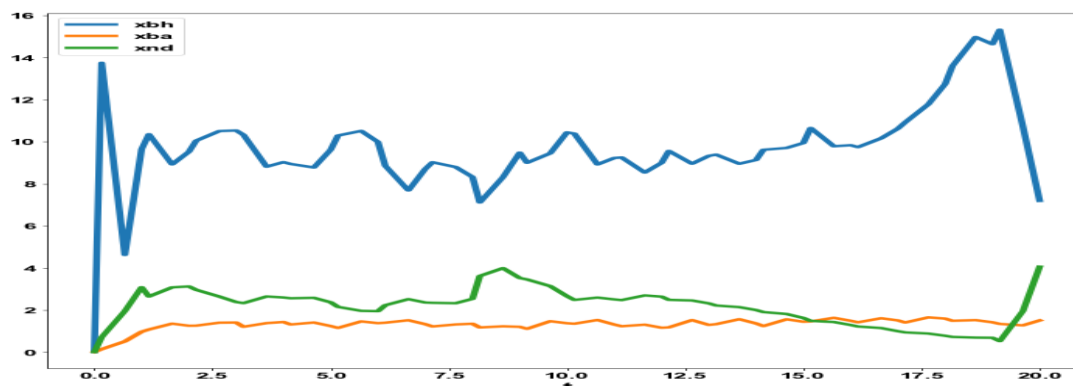


Figure 3d: XBH, XBA, XND profile MNLMPc soluble material concentration minimization

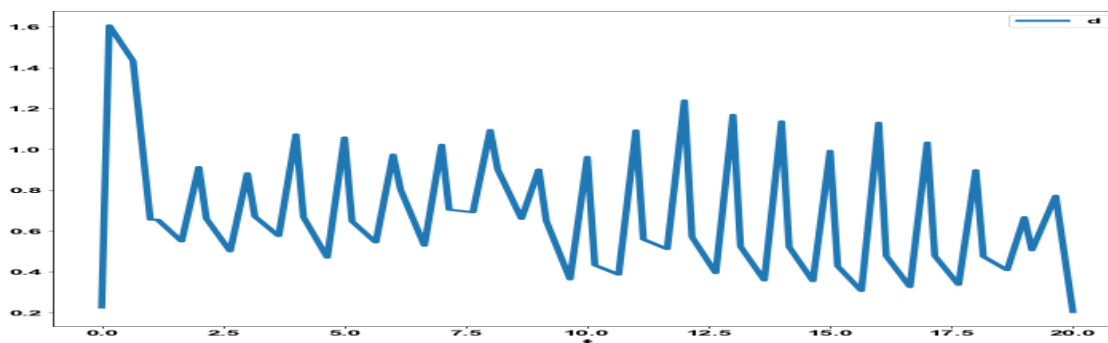


Figure 3e: dilution rate MNLMPc soluble material concentration minimization

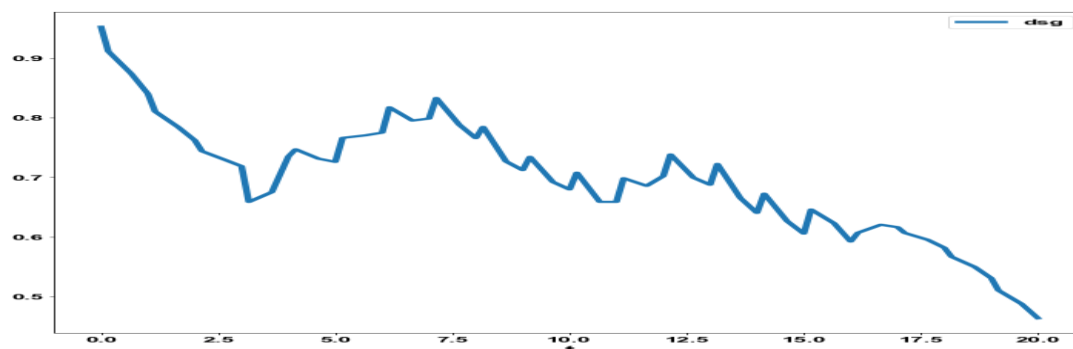


Figure 3f: dilution rate (with Savitzky Golay filter) MNLMPc soluble material concentration minimization

In the third case, In the second case, the variables representing the soluble materials (soluble nitrate and nitrite nitrogen, soluble ammonium nitrogen, and soluble biodegradable organic material) and the particulate variables (active heterotrophic particulate mass, active autotrophic particulate mass,

and particulate biodegradable organic nitrogen) were clubbed together as

S_{total} and X_{total} . In this case, $\sum_{t_i=0}^{t_i=t_f} S_{total}(t_i)$, $\sum_{t_i=0}^{t_i=t_f} X_{total}(t_i)$ was

minimized individually, leading to values of 10.8079 and 0.01647. The

overall optimal control problem will involve the minimization of

$$\left(\sum_{t_i=0}^{t_i=t_f} S_{total}(t_i) - 10.8079 \right)^2 + \left(\sum_{t_i=0}^{t_i=t_f} X_{total}(t_i) - 0.01647 \right)^2 \quad \text{was}$$

minimized subject to the equations governing the model. This led to a value of zero (the Utopia solution). The various concentration profiles for this MNLMPC calculation are shown in Figs. 4a-4d. The obtained control profile

of s exhibited noise (Fig. 4e). This was remedied using the Savitzky-Golay Filter. The smoothed-out version of this profile is shown in Fig. 4f.

In all the cases, the MNLMPC calculations converged to the Utopia solution, validating the analysis of Sridhar (2024), which showed that the presence of a limit or branch point enables the MNLMPC calculations to reach the best possible (Utopia) solution.

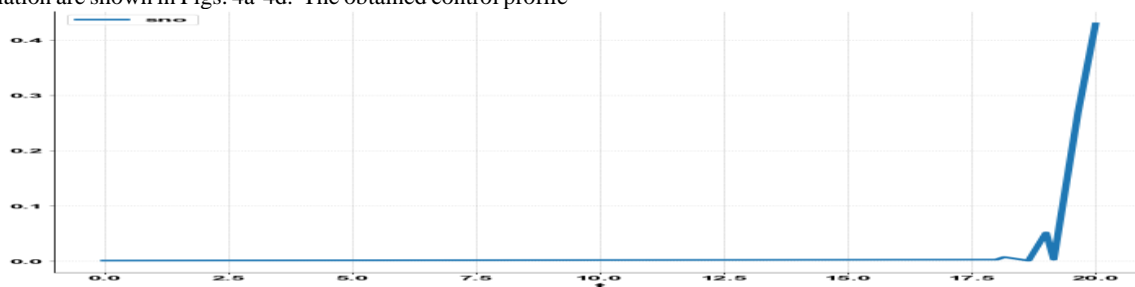


Figure 4a: SNO profile MNLMPC X and S concentration minimization

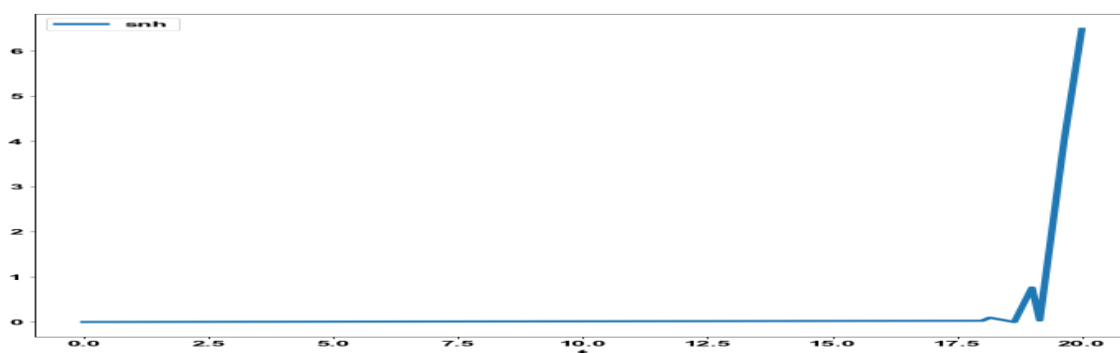


Figure 4b: SNH profile MNLMPC X and S concentration minimization

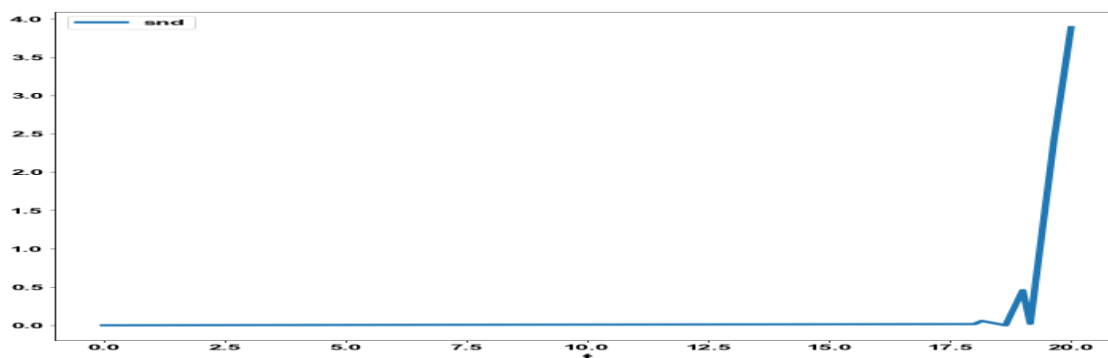


Figure 4c: SND profile MNLMPC X and S concentration minimization

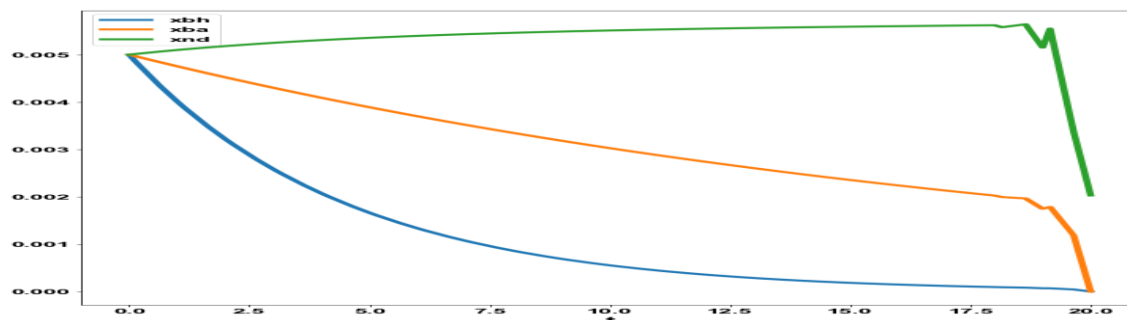


Figure 4d: XBH, XBA, XND profile MNLMPC X and S concentration minimization

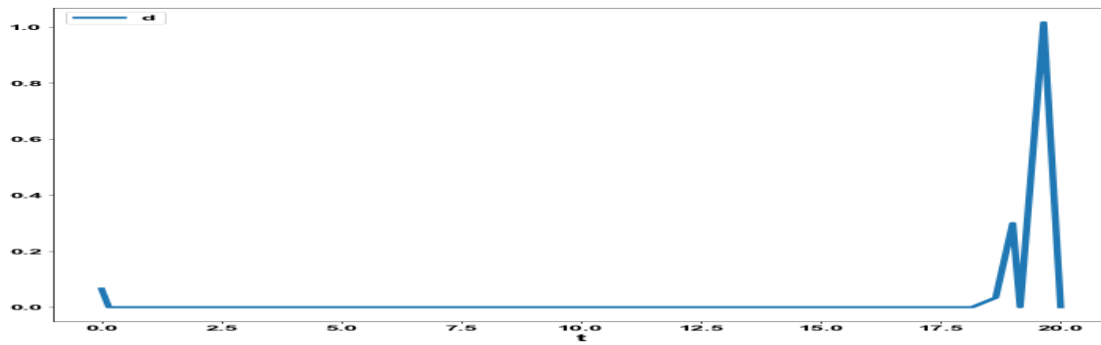


Figure 4e: dilution rate MNLMPX and S concentration minimization

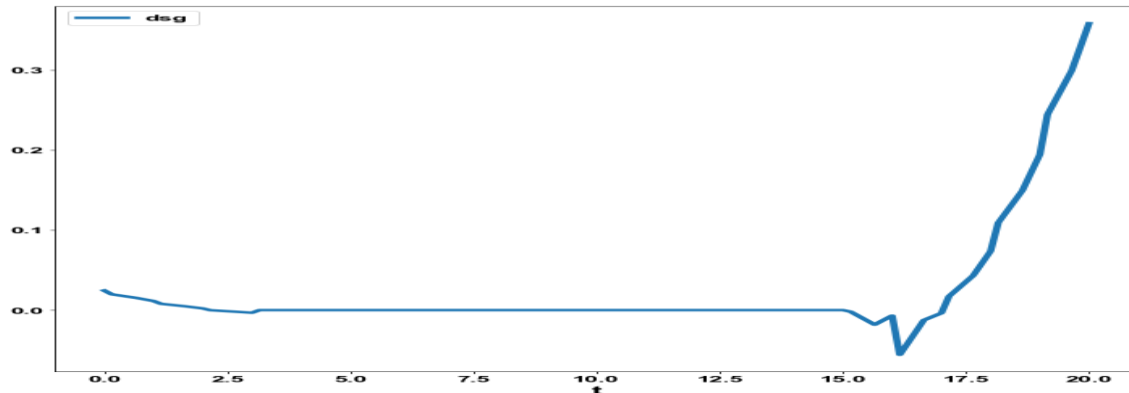


Figure 4f: dilution rate (with Savitzky Golay filter) MNLMPX and S concentration minimization

Conclusions

Bifurcation analysis and Multiobjective nonlinear model predictive control calculations were performed on the activated sludge model (ASM1). The bifurcation analysis revealed the existence of branch points. The branch points (which produced multiple steady-state solutions originating from a singular point) are very beneficial as they caused the multiobjective nonlinear model predictive calculations to converge to the Utopia point (the best possible solution) in both models. A combination of bifurcation analysis and multiobjective nonlinear model predictive control for the activated sludge model (ASM1) 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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