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Analysis and Control of Water Pollution Models

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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 (MNLMPC) 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 MNLMPC 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

Schwarzenbach et al. (2010) [1] investigated the connection between global water pollution and human health. Shah et al. (2018) [2] performed optimal control studies for the transmission of water pollutants. Guo et al (2019) [3] worked on mathematical modelling and application for simulation of water pollution accidents. Bonyah et al (2021) [4] studied water pollution transmission. Issakhov et al (2023) [5], performed numerical modeling studies of water pollution by products of chemical reactions from the activities of industrial facilities at variable and constant temperatures of the environment. Sabir et al (2023) [6] researched the numerical performance of the novel fractional water pollution model through the Levenberg-Marquardt backpropagation method. Anjam et L (2023) [7] analyzed a fractional pollution model in a system of three interconnecting lakes. Yang et al (2023) [8] investigated the prediction and control of water quality in a recirculating aquaculture system based on hybrid neural network. Mousavi et al (2023) [9] performed system dynamics modeling for effective strategies in water pollution control: insights and applications. Batabyal et al (2024) [10] compared the decentralized and centralized water pollution cleanup in the Ganges in a model with three cities. Ebrahimzadeh et al (2024) [11] studied the water pollution management through a comprehensive fractional modeling framework and optimal control Techniques.

This paper aims to perform bifurcation analysis in conjunction with multiobjective nonlinear model predictive control (MNLMPC) for two water pollution models Shah et al (2018) [2] (Model 1) and Ebrahimzadeh et al (2024) [11] (Model 2). This paper is organized as follows. First, the model equations are presented. The numerical procedures (bifurcation analysis and multiobjective nonlinear model predictive control (MNLMPC) are then described. This is followed by the results and discussion, and conclusions.

Model equations

For Model 1(Shah et al (2018) [2]), the model equations are

$$\begin{aligned}
\frac{d(wval)}{dt} &= b-\left(\beta_1 wval(sval)\right)-\left(\beta_2 wval(ival)\right)+\left(\varepsilon\beta_2 ival\right)-\left((\mu)wval\right)\\
\frac{d(sval)}{dt} &= \left(\beta_1 wval(sval)\right)+\delta u_1(ival)-(\mu)sval\\
\frac{d(ival)}{dt} &= \left(\beta_2 wval(ival)\right)-\left(\varepsilon\beta_2 ival\right)-(\delta+u_1)ival-(\mu)ival
\end{aligned} \quad (1)$$

The base parameters are

$$b=0.7;\beta_1=0.18;\beta_2=0.02;\delta=0.3;\varepsilon=0.1;\mu=0.4;u1=1;$$

In this model, β_2 is the bifurcation parameter and u1 is the control variable.

For Model 2Ebrahimzadeh et al (2024) [11], the model equations are

$$\frac{d(wval)}{dt} = \Lambda - (\alpha_1 wval(sval)) - (\alpha_2 wval(ival)) + (\rho\alpha_2 ival) - ((\mu)wval)$$
$$\frac{d(sval)}{dt} = (\alpha_1 wval(sval)) + \delta uval(ival) - (\theta_1 + \mu)sval \quad (1)$$
$$\frac{d(ival)}{dt} = (\alpha_2 wval(ival)) - (\rho\alpha_2 ival) - (\delta + uval + \theta_2 + \mu)ival$$
$$\frac{d(tval)}{dt} = (\theta_1)sval + (\theta_2)ival - (\mu)tval$$

Here *wval* represents the number of polluted water sources, *sval* is the water sources prone to pollution, *ival* is the water sources infected by pollutants, and *tval* describes the number

of water sources that have been recovered from the insoluble class due to treatment.

The base parameter values are uval is the bifurcation parameter and the control variable.

$$\Lambda = 0.8, \rho = 0.25, \alpha_1 = 0.18, \alpha_2 = 0.02, \delta = 0.3, \mu = 0.4,$$
$$\theta_1 = 0.2, \theta_2 = 0.5, uval = 0.99.$$

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[12]; Dhooge Govearts, Kuznetsov, Mestrom and Riet, 2004[13]). 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 $w = [w_1, w_2, w_3, w_4, ...w_{n+1}]$ must satisfy $Aw = 0$ (3)

Where A is

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

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,

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

@ 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[14]; 2009[15]) and Govaerts [2000] [16]

Multiobjective Nonlinear Model Predictive Control (MNLMPC)

Flores Tlacuahuaz et al (2012) [17] developed a multiobjective nonlinear model predictive control (MNLMPC) method that is rigorous and does not involve weighting functions or additional constraints. This procedure is used for performing the MNLMPC 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 MNLMPC 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

$$\min\left(\sum_{j=1}^{n}\left(\sum_{t_{i=0}}^{t_i=t_f} q_j(t_i) - q_j^*\right)\right)^2$$
$$subject\ to\ \frac{dx}{dt} = F(x,u); \quad (7)$$

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) [18] 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) [19]and confirmed as a global solution with BARON (Tawarmalani, M. and N. V. Sahinidis 2005) [20].

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 $\left(\sum_{j=1}^{n}\left(\sum_{t_{i=0}}^{t_i=t_f} q_j(t_i) - q_j^*\right)\right)^2$ 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 Utopia point is when $\sum_{t_{i=0}}^{t_i=t_f} q_j(t_i) = q_j^*$ for all j.

Sridhar (2024) [21] 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) [22]. 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 MNLPMC calculations will minimize the function $(q_1 - q_1^*)^2 + (q_2 - q_2^*)^2$. The multi-objective optimal control problem is

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

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

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

the optimal control co-state equation (Upreti; 2013) [25] 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

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

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

For model 1, the bifurcation analysis with β_2 as the bifurcation parameter, revealed the existence of a branch point at (*wval, sval, ival,* β_2) values of (1.75, 0, 0, 1.0303). This is shown in Fig. 1.

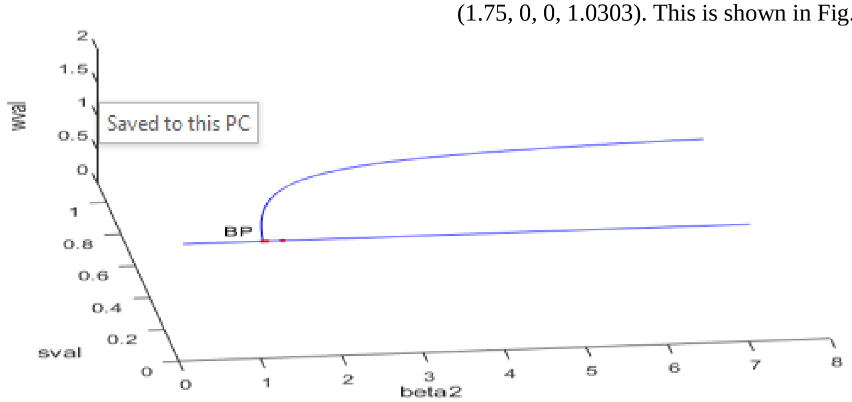

Figure 1: Bifurcation analysis for model 1

For the MNLMPC calculations, $\sum_{t_i=0}^{t_i=t_f} wval(t_i), \sum_{t_i=0}^{t_i=t_f} sval(t_i), \sum_{t_i=0}^{t_i=t_f} ival(t_i)$ were minimized individually and led to values of 1.75, 0, and 0. u1 is the control parameter. The multiobjective optimal control problem will involve the minimization of

$$(\sum_{t_i=0}^{t_i=t_f} wval(t_i) - 1.75)^2 + (\sum_{t_i=0}^{t_i=t_f} ival(t_i) - 0)^2 + (\sum_{t_i=0}^{t_i=t_f} sval(t_i) - 0)^2$$

subject to the equations governing the model. This led to a value of zero (the Utopia solution. The MNLMPC control value of obtained for u1 is was 0.284338. The various MNLMPC profiles are shown in Figures 2-5. The MNLMPC calculations converged to the Utopia solution, validating the analysis by Sridhar (2024) [21], which demonstrated that the presence of a limit point/branch point enables the MNLMPC calculations to reach the optimal (Utopia) solution.

When bifurcation analysis was performed on Model 2, with uval is bifurcation parameter, two branch points were obtained at (*wval, sval, ival, tval,uval*) values of (2.0, 0.0, 0.0, 0.0 -1.1650) and (3.33; -0.88, 0.0, -0.44, -1.1383). This is shown in Fig. 6. For the MNLMPC calculations,

$\sum_{t_i=0}^{t_i=t_f} wval(t_i), \sum_{t_i=0}^{t_i=t_f} sval(t_i), \sum_{t_i=0}^{t_i=t_f} ival(t_i)$ were minimized individually and led to values of 2, 0, and 0.

$\sum_{t_i=0}^{t_i=t_f} tval(t_i)$ was maximized and led to a value of 2. The multiobjective optimal control problem will involve the minimization of

$$(\sum_{t_i=0}^{t_i=t_f} wval(t_i) - 2)^2 + (\sum_{t_i=0}^{t_i=t_f} tval(t_i) - 2)^2 + (\sum_{t_i=0}^{t_i=t_f} ival(t_i) - 0)^2 + (\sum_{t_i=0}^{t_i=t_f} s$$

subject to the equations governing the model. This led to a value of zero (the Utopia solution. The MNLMPC control value of obtained for uval was 0.11714. The various MNLMPC profiles are shown in Figures 7-11. The MNLMPC calculations converged to the Utopia solution, validating the analysis by Sridhar (2024) [21], which demonstrated that the presence of a limit point/branch point enables the MNLMPC calculations to reach the optimal (Utopia) solution.

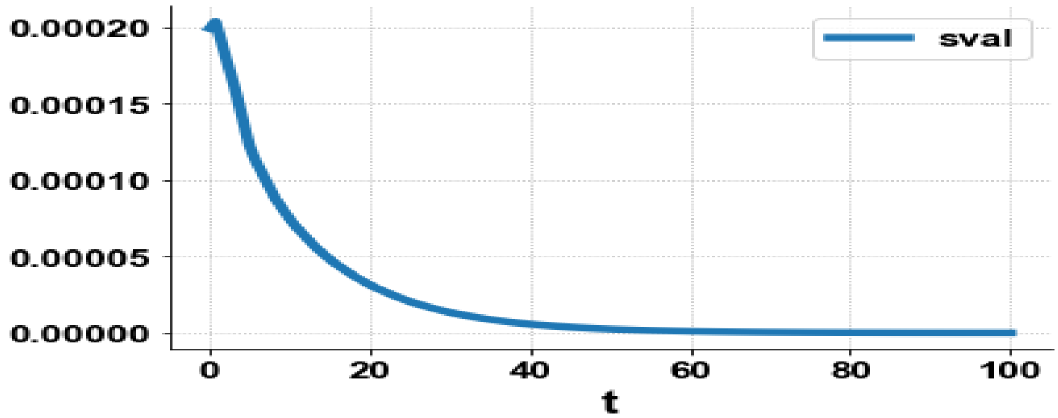

Figure 2: MNLMPC for model 1 sval vs t

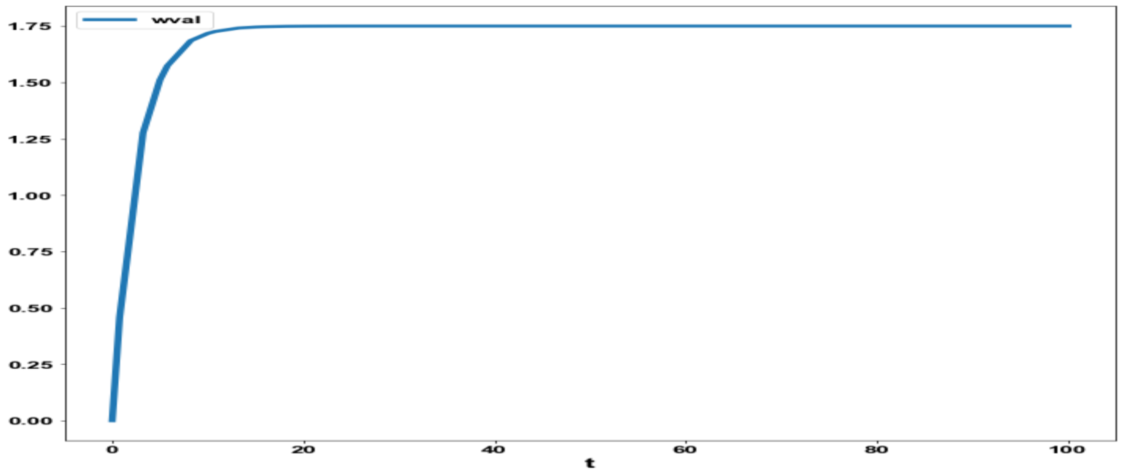

Figure 3: MNLMPC for model 1 wval vs t

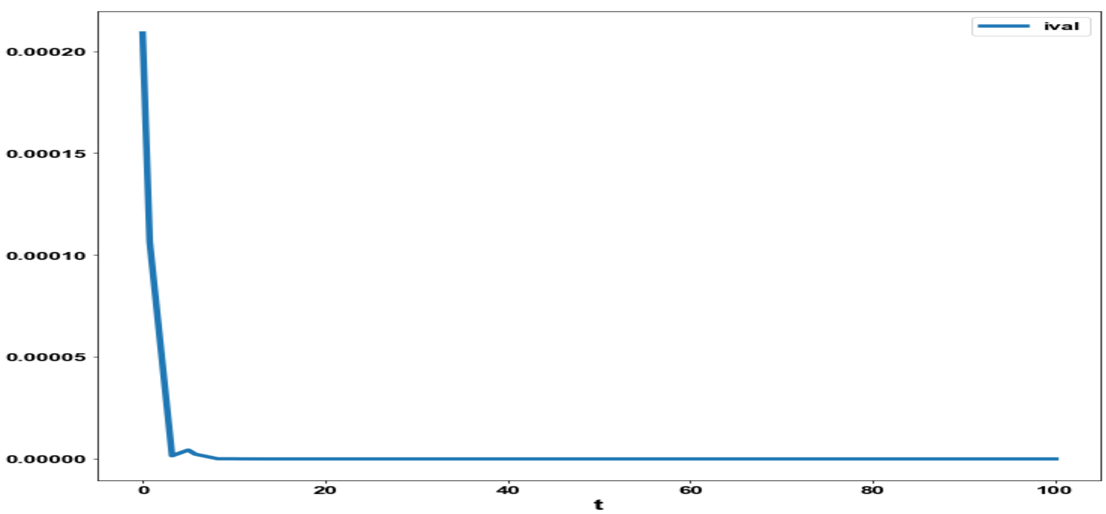

Figure 4: MNLMPC for model 1 ival vs t

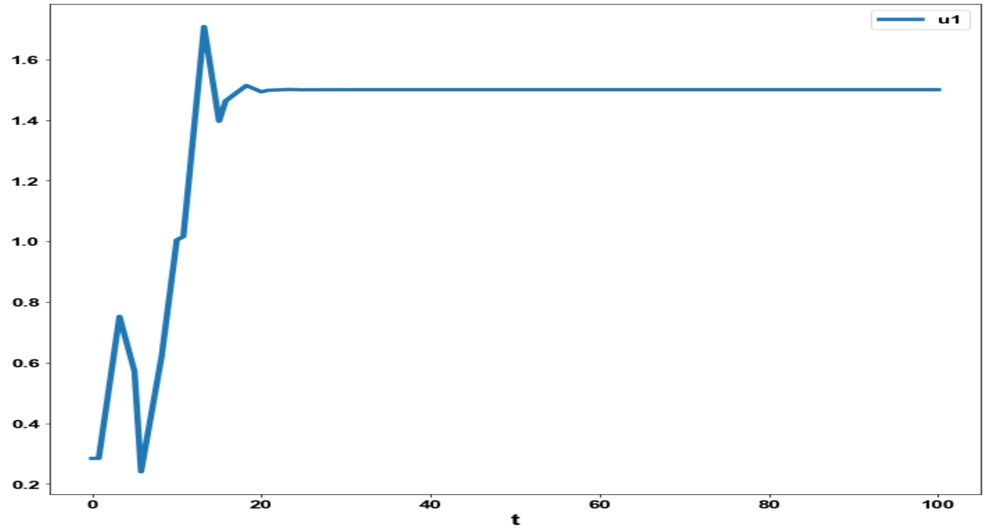

Figure 5: MNLMPC for model 1 u1 vs t

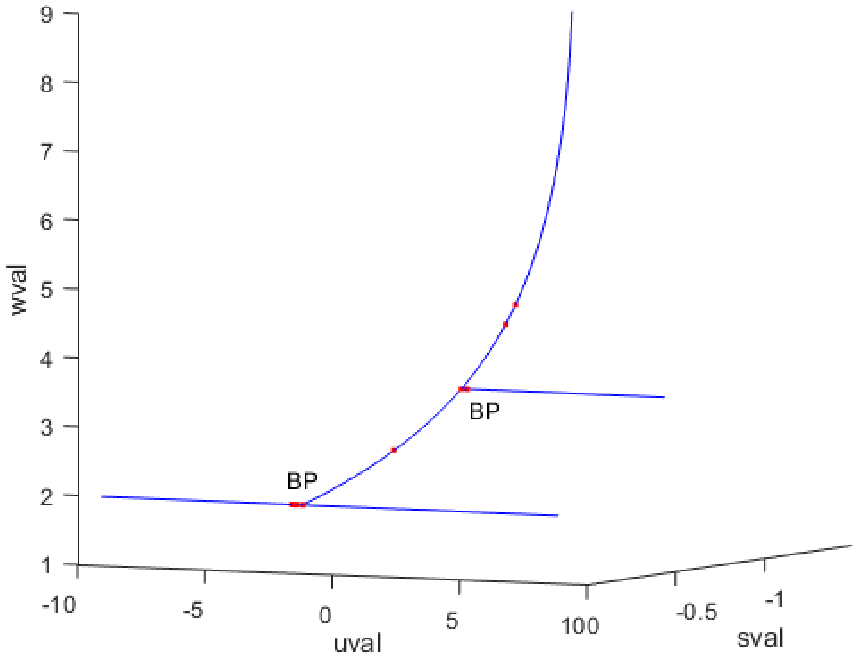

Figure 6: Bifurcation analysis for model 2

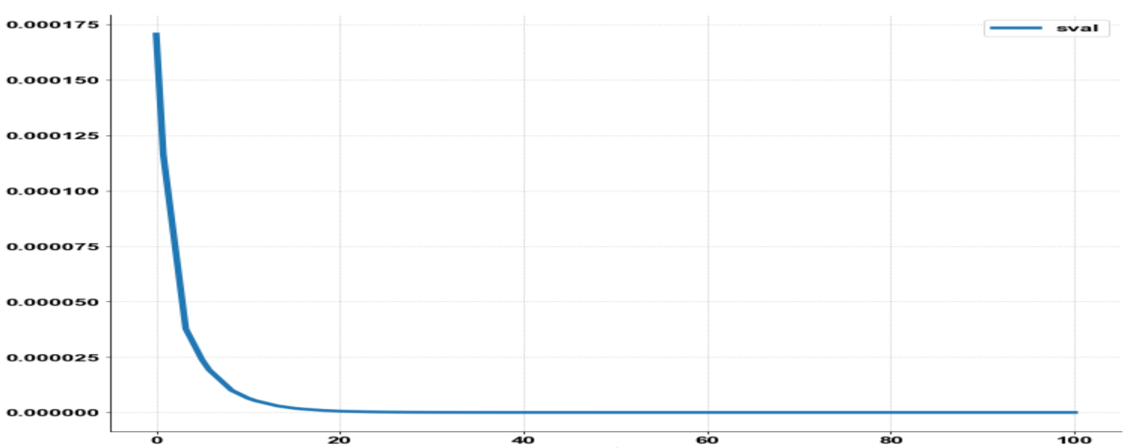

Figure 7: MNLMPC for model 2 sval vs t

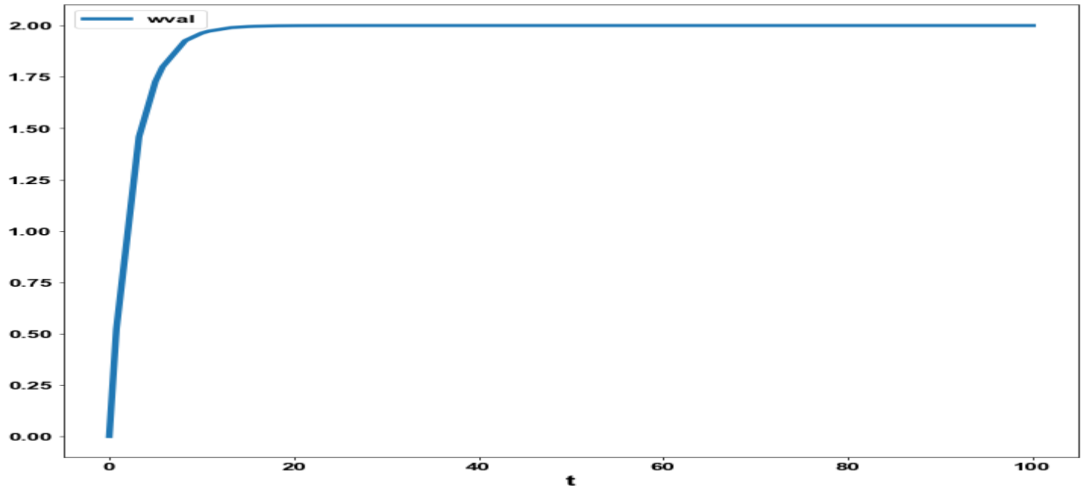

Figure 8: MNLMPC for model 2 wval vs t

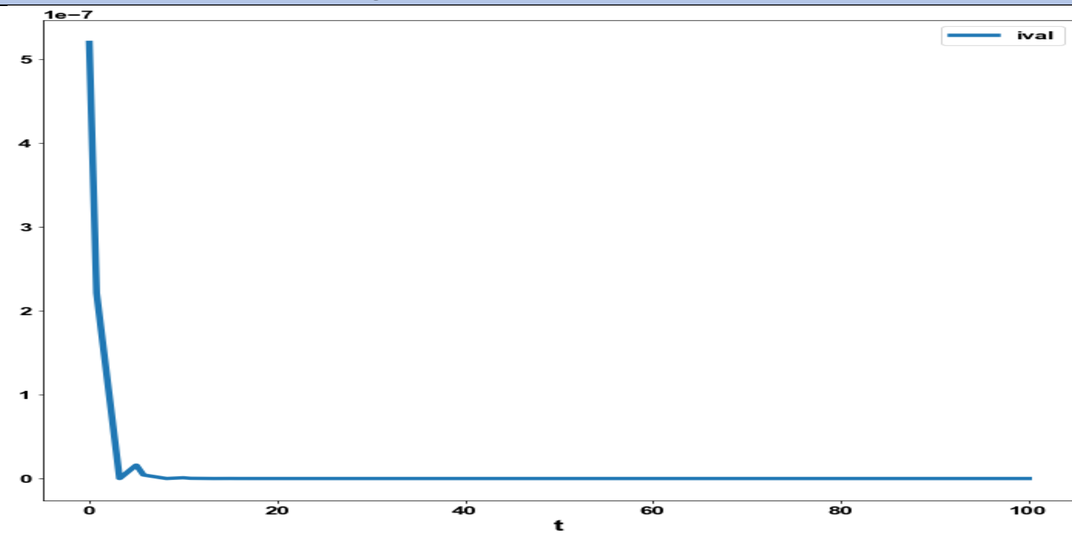

Figure 9: MNLMPC for model 2 ival vs t

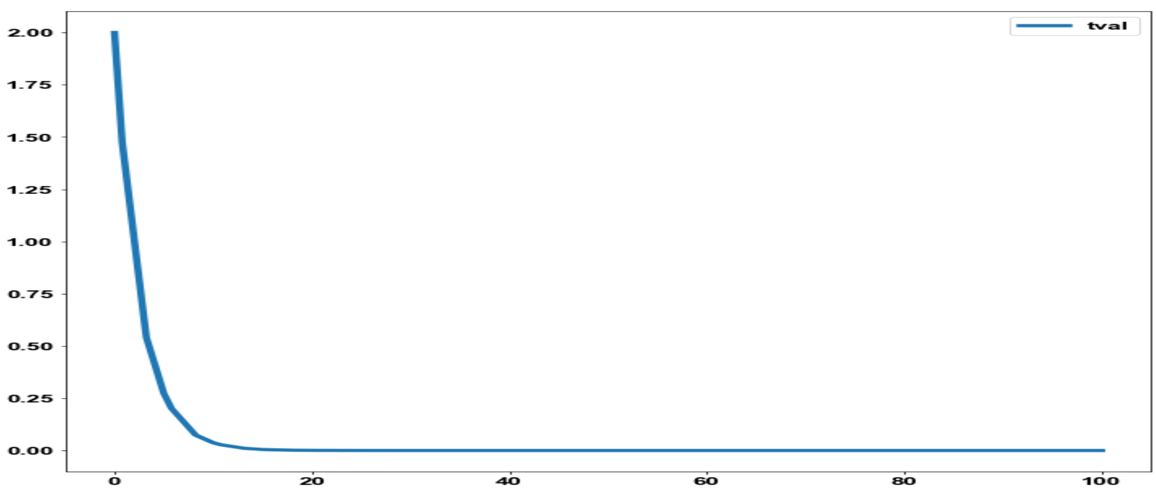

Figure 10: MNLMPC for model 2 tval vs t

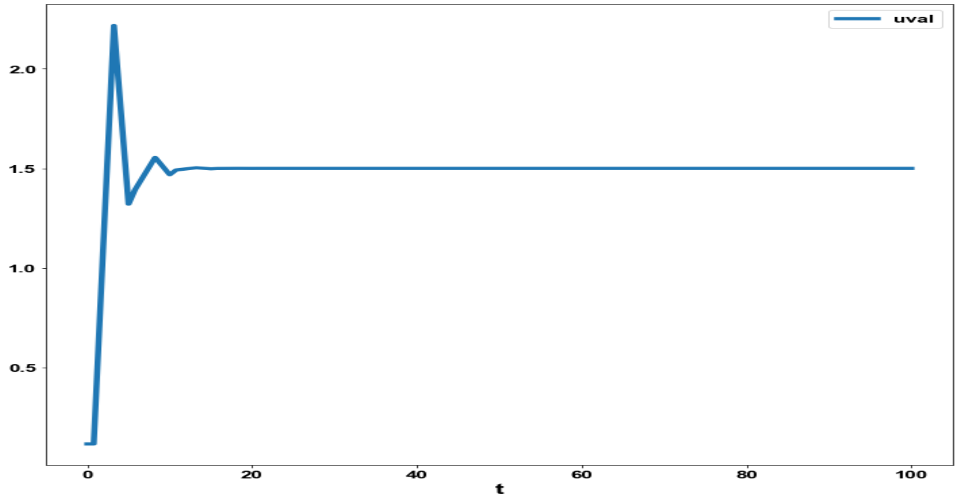

Figure 11: MNLMPC for model 2 uval vs t

Conclusions

Bifurcation analysis and Multiobjective nonlinear model predictive control calculations were performed on two water pollution models. The bifurcation analysis revealed the existence of a branch points in both models. The branch points (which causes 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 models. A combination of bifurcation analysis and Multiobjective Nonlinear Model Predictive Control (MNLMPC) for dynamic models involving water pollution 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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