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Analysis and control of a carbon dioxide removal model

Lakshmi Narayan Sridhar

Chemical Engineering Department, University of Puerto Rico, Mayaguez, Puerto Rico.
Email: lakshmin.sridhar@upr.edu

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ABSTRACT

Carbon dioxide removal from the atmosphere has emerged as one of the most critical strategies in responding to the accelerating climate crisis. It is important to develop rigorous and beneficial strategies and take steps to remove carbon dioxide from the atmosphere. In this study, bifurcation analysis and multi-objective nonlinear model predictive control are performed on a carbon dioxide removal model. Bifurcation analysis is a powerful mathematical tool used to address the nonlinear dynamics of various processes. 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 conducted using the optimization language PYOMO in conjunction with state-of-the-art global optimization solvers IPOPT and BARON. The bifurcation analysis revealed the existence of limit points. The MNLMPC converged to the Utopia solution. The limit points, which cause multiple steady-state solutions from a singular point, are highly beneficial because they enable the multi-objective nonlinear model predictive control calculations to converge to the Utopia point, representing the best possible solution in the model.

Contribution/Originality: The originality of this work lies in the integration of bifurcation analysis and optimal control of the carbon dioxide removal process. Such an integration has not been previously accomplished.

1. INTRODUCTION

While reducing emissions at their sources remains essential, decades of accumulated greenhouse gases have pushed atmospheric CO_2 concentrations to levels that continue to warm the planet, even with improved mitigation efforts. As a result, scientists, engineers, policymakers, and communities are increasingly exploring techniques to actively draw carbon dioxide out of the atmosphere and store it in stable, long-term reservoirs. The goal is not to replace emissions reductions but to complement them, especially in sectors where complete decarbonization remains technologically or economically challenging. Understanding the scientific basis, technological options, ecological considerations, and socio-economic implications of CO_2 removal is therefore vital in shaping a balanced and effective climate strategy for future generations.

Natural processes of carbon sequestration form the foundation for many approaches to removing CO_2 from the atmosphere. Forests, soils, oceans, and wetlands already serve as substantial carbon sinks, absorbing significant amounts of carbon dioxide through photosynthesis and biological activity. Reforestation and afforestation are often viewed as straightforward methods for enhancing natural sinks, as growing trees capture CO_2 and store it in biomass. Similarly, soil carbon sequestration through practices such as no-till agriculture, cover cropping, rotational grazing, and organic soil amendments can increase the amount of carbon stored in soils. These techniques are appealing due to their relative simplicity and additional ecological benefits, including improved biodiversity, increased water retention, and reduced soil erosion. However, natural sinks can become saturated over time, and their permanence remains uncertain, as carbon stored in vegetation can be released through fires, disease, or land-use changes, and soil carbon can be lost if management practices shift. Therefore, while natural pathways are valuable, they are not sufficient on their own to counterbalance ongoing anthropogenic emissions.

Ocean-based carbon removal strategies also leverage natural processes, as oceans already absorb about a quarter of annual human CO_2 emissions. Proposed techniques include ocean fertilization, which introduces nutrients like iron to stimulate phytoplankton growth, thereby increasing carbon uptake through photosynthesis. Enhanced alkalinity approaches aim to accelerate natural geological processes that regulate ocean chemistry by adding finely ground minerals such as olivine, which react with CO_2 and store it in the ocean for millennia. Seaweed cultivation has also garnered interest, as large-scale kelp farming could capture carbon, with long-term storage achieved by sinking the biomass to deep ocean layers. Despite these promising ideas, concerns remain regarding ecological impacts, such as potential disruptions to marine food webs, alterations in ocean chemistry, and unintended biodiversity loss. These uncertainties highlight the necessity for extensive research before deploying ocean-based CO_2 removal at significant scales.

Technological or engineered carbon removal methods represent another major pathway, offering the advantage of greater controllability, measurability, and durability compared to some biological methods. Direct air capture is one of the most publicized technologies, utilizing chemical sorbents or solid materials to bind CO_2 from ambient air. Once captured, the carbon dioxide can be compressed and either stored in deep geological formations or utilized in industrial processes. Direct air capture systems can theoretically scale to remove millions of tons of CO_2 annually and provide highly durable storage when paired with geological sequestration. Nonetheless, these systems are energy-intensive and currently expensive, raising questions about the feasibility of large-scale deployment without significant improvements in efficiency and reductions in cost. Another engineered approach is bioenergy with carbon capture and storage, which involves growing biomass, using it to produce energy, and capturing and storing the resulting CO_2 emissions. If sustainably implemented, this system can yield net-negative emissions, although concerns about land competition, water usage, and impacts on food systems must be addressed.

Mineralization, or enhanced weathering, is rooted in geological processes that naturally remove CO_2 from the atmosphere over millions of years. By accelerating the exposure of certain reactive rocks to atmospheric CO_2, the gas can be transformed into stable carbonate minerals. Spreading finely crushed basalt or olivine on agricultural lands is one method under investigation, as is carbon injection into ultramafic rock formations where rapid mineralization can occur underground. This method promises extremely durable storage with minimal risk of leakage. However, large-scale mining, grinding, and distribution of minerals require substantial energy, infrastructure, and land-use considerations, raising concerns about environmental footprints and economic viability.

One of the most overlooked aspects of CO_2 removal is the need to integrate these various methods into broader climate strategies that account for economics, social equity, and governance. Carbon removal cannot be viewed simply as a technical problem; it also has profound implications for land management, community livelihoods, environmental justice, and geopolitical cooperation. Large-scale afforestation, for example, may compete with agricultural land, affecting food prices and rural communities. Likewise, engineered solutions may concentrate infrastructure in certain regions, prompting discussions about who bears the risks, who benefits, and how costs are shared. Transparent governance frameworks, community participation, and international coordination are essential to ensure that CO_2 removal is pursued ethically, responsibly, and effectively.

Another key element is the importance of monitoring, reporting, and verification. For carbon removal to contribute meaningfully to climate goals, accurate measurement of carbon flows and storage durability is essential. Natural sinks require continual monitoring to ensure that captured carbon remains stored, while engineered methods demand rigorous oversight to confirm that removal processes are truly net-negative once all energy and material inputs are accounted for. Advances in remote sensing, geochemical monitoring, and digital tracking are helping improve transparency and reliability, but challenges remain in standardizing measurement techniques across different removal pathways.

Economic incentives will also shape the future of carbon dioxide removal. Carbon markets, climate finance mechanisms, and government subsidies can either accelerate or hinder adoption. Currently, the high cost of many engineered approaches limits widespread implementation, but investment in research, development, and deployment may reduce costs over time, much like renewable energy technologies have become more affordable. Policy support, such as tax credits for carbon storage or procurement programs for net-negative products, may play a significant role in building early markets. Ensuring that policies do not inadvertently encourage excessive reliance on carbon removal at the expense of emissions reduction is also critical, as removal must complement rather than replace decarbonization efforts.

The global scale of the climate challenge means that no single CO_2 removal strategy can solve the problem alone. Instead, a diversified portfolio of approaches, tailored to specific regions, ecosystems, and economic contexts, will likely be necessary. Nations with vast forested areas may prioritize reforestation and soil carbon enhancement, while regions with strong renewable energy capacity might invest more in direct air capture. Coastal nations could explore seaweed cultivation or enhanced ocean alkalinity, though only after careful ecological assessment. Matching solutions to local conditions can help maximize effectiveness while minimizing unintended consequences.

Carbon dioxide removal is not a silver bullet but a critical component of a multifaceted climate response. It offers a means to draw down excess CO_2 that would otherwise remain in the atmosphere for centuries, thereby slowing global warming and reducing long-term climate risks. Balancing natural and engineered approaches, improving scientific understanding, developing supportive yet responsible policy frameworks, and ensuring equitable implementation are all essential to realizing the potential of CO_2 removal. As the world continues to grapple with the realities of climate change, building the capacity to remove and responsibly store carbon will become an increasingly important tool in safeguarding environmental stability and human well-being for future generations.

Resnik et al. [1] discussed the aqua ammonia process for simultaneous removal of CO_2, SO_2, and NOx. Rao and Rubin [2] identified cost-effective CO_2 control levels for amine-based CO_2 capture systems. Robinson et al. [3] investigated the environmental effects of increased atmospheric carbon dioxide. Stolaroff et al. [4] researched carbon dioxide capture from atmospheric air using sodium hydroxide spray. Mahmoudkhani and Keith [5] performed a thermodynamic analysis of low-energy sodium hydroxide recovery for CO_2 capture from atmospheric air. Kamarudin et al. [6] investigated the removal of carbon dioxide using a water-in-oil emulsion liquid membrane containing triethanolamine. Pellegrini et al. [7] conducted a comparative study of chemical absorbents in post-combustion CO_2 capture. Niu et al. [8] performed experimental studies and rate-based process simulations of CO_2 absorption with aqueous ammonia solutions. Choi et al. [9] investigated the influence of operating temperature on the CO_2 - NH_3 reaction in an aqueous solution. Gao et al. [10] showed that the rising CO_2 and increased light exposure synergistically reduce marine primary productivity. Darde et al. [11] performed a process simulation of CO_2 capture with aqueous ammonia using the extended UNIQUAC model. Jiang et al. [12] conducted experimental studies on the influence of HCO_3 on the absorption and desorption of CO_2 from ammonia solution. Chen et al. [13] and Chen et al. [14] studied the interaction of droplets with carbon dioxide. Han et al. [15] calculated the liquid phase mass transfer coefficient of carbon dioxide absorption by a water droplet. Kale et al. [16] modelled the reactive absorption of CO_2 using monoethanolamine. Voice et al. [17] used aqueous 3-(methylamino) propylamine for CO_2 capture. Yoo et al. [18] studied the carbon dioxide capture capacity of sodium hydroxide aqueous solution. Zhang and Guo [19] performed process simulations of large-scale CO_2 capture in coal-fired power plants using aqueous ammonia solution. Sundar et al. [20] modelled the dynamics of carbon dioxide removal in the atmosphere.

This work involves bifurcation analysis and multiobjective nonlinear model predictive control applied to a dynamic model describing carbon dioxide removal from the atmosphere [20]. 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 and discussion are then provided, culminating in the conclusions.

1.1. Model Equations

In this model, cv is the cumulative concentration of carbon dioxide, av is the concentration of externally introduced liquid species, cp is the density of particulate matter formed due to the interaction of carbon dioxide with liquid species, and cm is the concentration of a suitable absorbent. Q is the rate of discharge of carbon dioxide from various sources, $\delta 0$ the interaction coefficient of the depletion rate of cv. The depletion of carbon dioxide is directly proportional to a) the product of the carbon dioxide and the liquid species concentration, with the rate constant $\lambda 1$ and b) the product of the carbon dioxide and the absorbent concentration with the rate constant $\mu 1$**.** The rate of introduction of liquid species needed to reduce the carbon dioxide concentration is directly proportional to the difference between the cumulative cv and c0, the threshold concentration, with the proportionality constant λ. The rate of reduction of av is directly proportional to av, with a rate constant $\lambda 0$. θ is the rate at which particulate matter is formed in the atmosphere as a result of the interaction of carbon dioxide with liquid species, while $\theta 0$ is the natural depletion rate coefficient of the particulate matter. μ is the rate of inflow of absorbent in the absorption chamber. $\mu 1$ The interaction coefficient of the natural depletion rate of cm is $\mu 0$. The differential equations are

$$\begin{aligned}
\frac{d(cv)}{dt} &= Q - \delta 0(cv) - \lambda 1(cv)av - mu1(cv)cm \\
\frac{d(av)}{dt} &= \lambda\left(cv - c0\right) - (\lambda 0)(av) - \lambda 1(cv)av \\
\frac{d(cp)}{dt} &= \theta(\lambda 1)(cv)av - (\theta 0)(cp) \\
\frac{d(cm)}{dt} &= \mu(cv) - \mu 0(cm) - \mu 1(cv)cm
\end{aligned} \tag{1}$$

The base model parameter values are

Q=1;$\delta 0$ =0.1;$\lambda 1$ =0.5;λ =0.4;$\lambda 0$ =0.2;θ =0.8;$\theta 0$ =0.7; c0=0.6;μ =1;$\mu 0$ =0.02; $\mu 1$ =0.6.

1.2. Bifurcation Analysis

The MATLAB software MATCONT is used to perform bifurcation calculations. Bifurcation analysis deals with multiple steady states and limit cycles. Multiple steady states occur because of the existence of branch points and limit points. Hopf bifurcation points cause the emergence of limit cycles. A commonly used MATLAB program that locates limit points, branch points, and Hopf bifurcation points is MATCONT [21]. This program detects limit points (LP), branch points (BP), and Hopf bifurcation points (H) for an ODE system.

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

$x \in R^n$ Let the bifurcation parameter be α . Since the gradient is orthogonal to the tangent vector,
The tangent plane at any point $w = [w_1, w_2, w_3, w_4, \ldots. w_{n+1}]$ must satisfy

$$Aw = 0 \tag{3}$$

Where A is

$$A = [\partial f/\partial x \quad |\partial f/\partial \alpha] \tag{4}$$

Where $\partial f/\partial x$ 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 $y = (y_1, y_2, y_3, y_4, \ldots y_n)$ must align with $\hat{w} = (w_1, w_2, w_3, w_4, \ldots w_n)$.

$$J\hat{w} = Aw = 0 \tag{5}$$

Since 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

$$\begin{aligned} Az &= 0 \\ Aw &= 0 \end{aligned} \tag{6}$$

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, for a branch point (BP), the matrix $B = \begin{bmatrix} A \\ w^T \end{bmatrix}$ must be singular.

At a Hopf bifurcation point,

$$det(2f_x(x, \alpha) @ I_n) = 0 \tag{7}$$

@ 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 [22], Kuznetsov [23], and Govaerts [24].

1.3. Multiobjective Nonlinear Model Predictive Control (MNLMPC)

The rigorous multiobjective nonlinear model predictive control (MNLMPC) method developed by Flores-Tlacuahuac et al. [25] was used.

Consider a problem where the variables $\sum_{t_{i=0}}^{t_i=t_f} q_j(t_i)$ (j=1, 2..n) have to be optimized simultaneously for a dynamic problem

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

t_f being the final time value, and n the total number of objective variables and u the control parameter. The single-objective optimal control problem is solved by individually 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 multi-objective optimal control (MOOC) problem that will be solved is described in detail.

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

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. [26] is used for these calculations. Here, the differential equations are converted into 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

1. Optimize $\sum_{t_i=0}^{t_i=t_f} q_j(t_i)$ and obtain q_j^*.
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 at 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 [29] demonstrated that when bifurcation analysis reveals the presence of limit and branch points, the MNLMPC calculations tend to converge to the Utopia solution. To achieve this, the singularity condition, caused by the presence of the limit or branch points, was imposed on the co-state equation [30]. 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 multiobjective optimal control problem is

$$min \quad (q_1 - q_1^*)^2 + (q_2 - q_2^*)^2 \quad subject\ to \quad \frac{dx}{dt} = F(x,u) \qquad (10)$$

Differentiating the objective function results in

$$\frac{d}{dx_i}((q_1 - q_1^*)^2 + (q_2 - q_2^*)^2) = 2(q_1 - q_1^*)\frac{d}{dx_i}(q_1 - q_1^*) + 2(q_2 - q_2^*)\frac{d}{dx_i}(q_2 - q_2^*) \qquad (11)$$

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

$$\frac{d}{dx_i}((q_1 - q_1^*)^2 + (q_2 - q_2^*)^2) = 0 \qquad (12)$$

The optimal control co-state equation [30] is

$$\frac{d}{dt}(\lambda_i) = -\frac{d}{dx_i}((q_1 - q_1^*)^2 + (q_2 - q_2^*)^2) - f_x\lambda_i; \quad \lambda_i(t_f) = 0 \qquad (13)$$

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

$$\frac{d}{dt}(\lambda_i) = -f_x\lambda_i; \lambda_i(t_f) = 0 \qquad (14)$$

At a limit or a branch point, for the set of ODEs $\frac{dx}{dt} = f(x,u)$ f_x is singular. Hence, there are two different vector 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 optimal solution is the utopia solution.

2. RESULTS AND DISCUSSION

When λ is the bifurcation parameter, a limit point was observed at (cv, av, cp, cm, λ) values of (0.307272 4.504612 0.790939 1.503559 -5.441899) (Figure 1a).

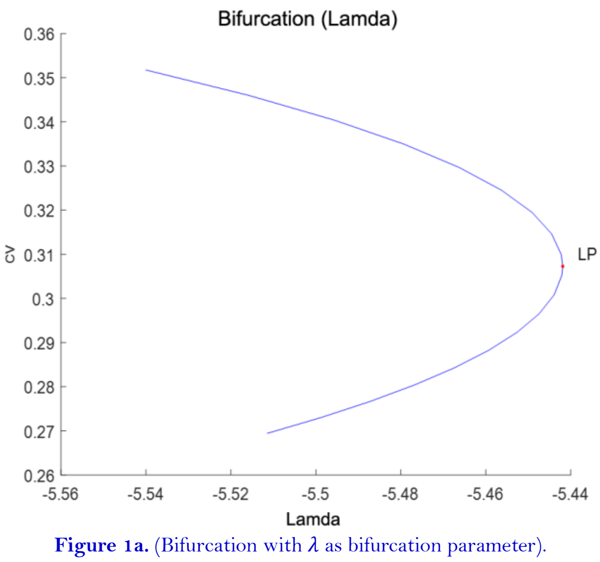

Figure 1a. (Bifurcation with λ as bifurcation parameter).

When $\lambda 0$ is the bifurcation parameter, a limit point was observed at (cv, av, cp, cm, $\lambda 0$) values of (0.647225 0.988076 0.365433 1.585034 -0.304495) (Figure 1b).

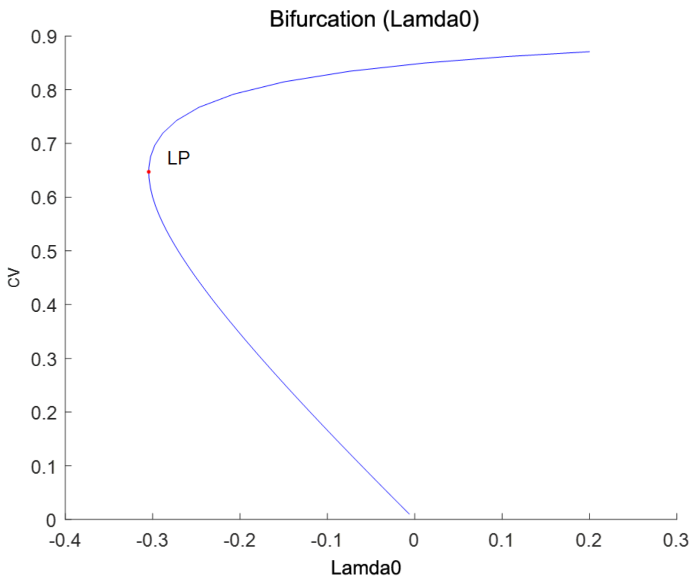

Figure 1b. (Bifurcation with $\lambda 0$ as bifurcation parameter).

When $\lambda 1$ is the bifurcation parameter, a limit point was observed at (cv, av, cp, cm, $\lambda 1$) values of (0.647224 -1.504323 0.365433 1.585034 -0.328413)(Figure 1c).

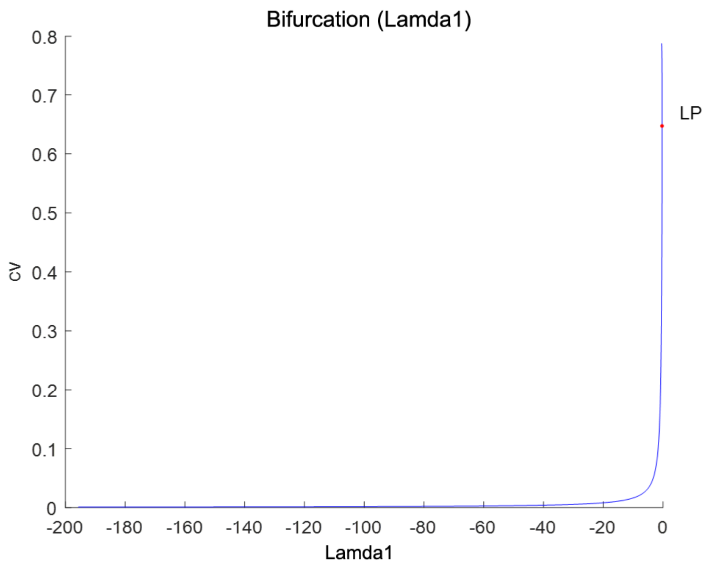

Figure 1c. (Bifurcation with $\lambda 1$ as bifurcation parameter).

When $\mu 0$ is the bifurcation parameter, a limit point was observed at (cv, av, cp, cm, $\mu 0$) values of (0.461101 -0.129043 -0.034001 3.555408 -0.146971) (Figure 1d).

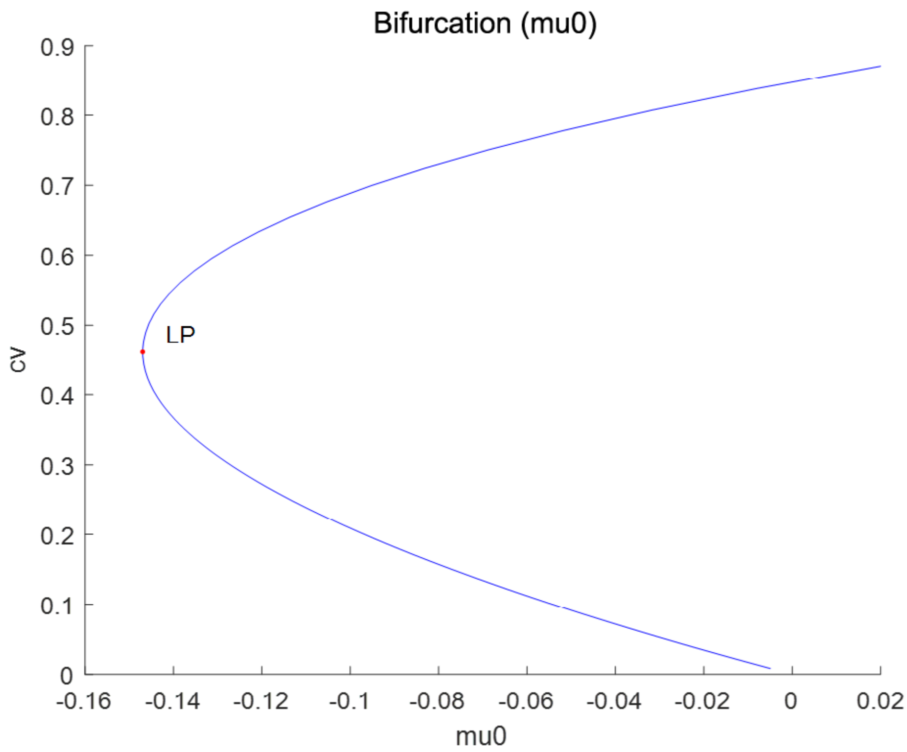

Figure 1d. (Bifurcation with $\mu 0$ as bifurcation parameter).

For the MNLMPCμ is the control parameter, and $(\sum_{t_i=0}^{t_i=t_f} cv(t_i)), (\sum_{t_i=0}^{t_i=t_f} av(t_i) + \sum_{t_i=0}^{t_i=t_f} cp(t_i))$ were minimized individually, and values of 0.26125 and 0. The overall optimal control problem will involve the minimization of $(\sum_{t_i=0}^{t_i=t_f} cv(t_i) - 0.26125)^2 + (\sum_{t_i=0}^{t_i=t_f} av(t_i) + \sum_{t_i=0}^{t_i=t_f} cp(t_i) - 0)^2$was minimized subject to the differential equations of the model. This led to a value of zero (the Utopia point). The MNLMPC values of the control variable μ is, 0.14187. The MNLMPC profiles are shown in Figures 2a-2c. The control profiles of the le exhibited noise, and this was remedied using the Savitzky-Golay filter to produce a smooth profile μsg (Figure 2c).

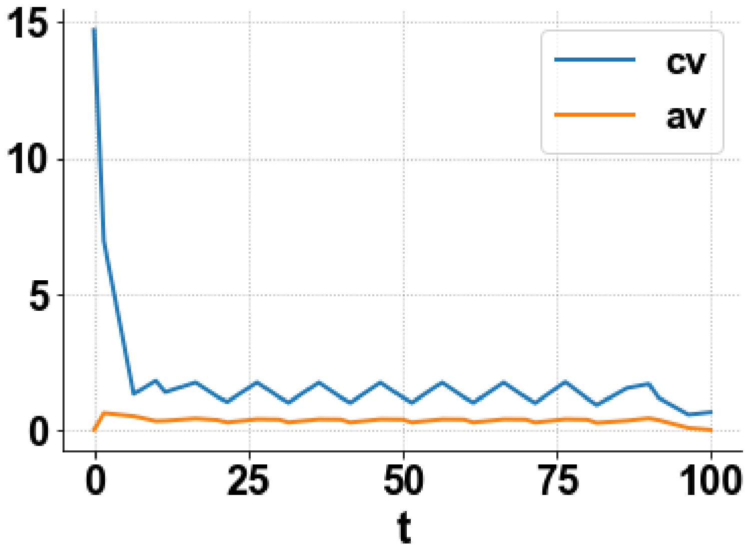

Figure 2a. MNLMPC cv, av profiles.

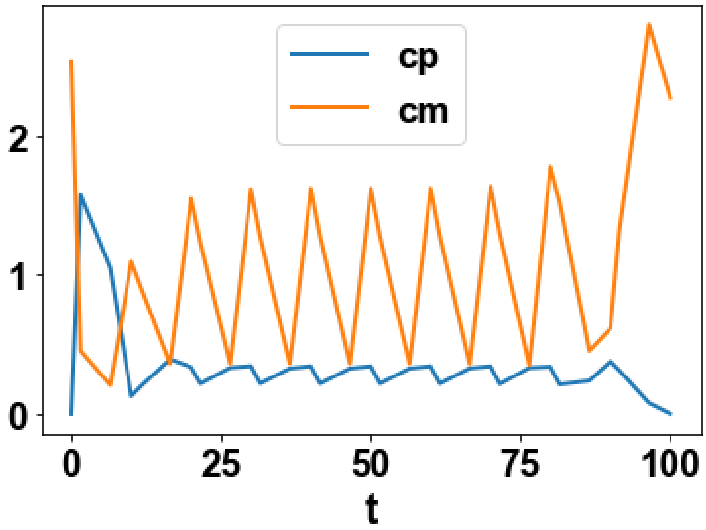

Figure 2b. MNLMPC cp, cm profiles.

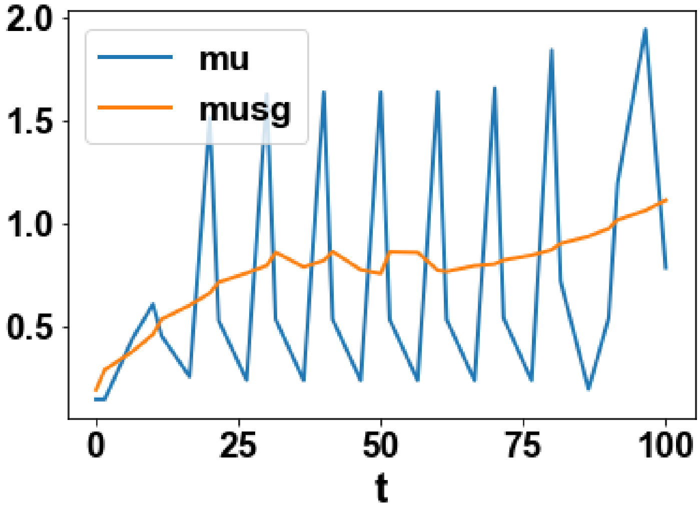

Figure 2c. MNLMPC MU, MUSG profiles.

The presence of limit points, even though they occur in infeasible regions where some variables have negative values, causes the MNLMPC calculations to converge to the Utopia solution, thereby validating the analysis in [29].

3. CONCLUSIONS

Bifurcation analysis and multiobjective nonlinear control (MNLMPC) studies on the carbon dioxide removal model. The bifurcation analysis revealed the existence of limit points. These limit points, which cause multiple steady-state solutions from a singular point, are highly beneficial because they enable the Multiobjective Nonlinear Model Predictive Control calculations to converge to the Utopia point the optimal solution in the models. The main contribution of this paper is the combination of bifurcation analysis and Multiobjective Nonlinear Model Predictive Control (MNLMPC) applied to a carbon dioxide removal model.

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Competing Interests: The author declares that there are no conflicts of interest regarding the publication of this paper.

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