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Vol: 3 & Iss: 3

Analysis and Control of a Dynamic Chemical Reactor Model

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Citation: Sridhar LN. Analysis and Control of a Dynamic Chemical Reactor Model. *J Petro Chem Eng* 2025;3(3):186-191.

Received: 22 September, 2025; **Accepted:** 24 September, 2025; **Published:** 26 September, 2025

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ABSTRACT

The dynamics of chemical reactors is highly nonlinear and multiple steady-states and liit ccles are observed. In this work, bifurcation analysis and multiobjective nonlinear model predictive control is performed on a dynamic chemical reactor model. 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 the existence of a Hopf bifurcation point and a limit point. The MNLMC converged to the utopia solution.The Hopf bifurcation point, which causes an unwanted limit cycle, is eliminated using an activation factor involving the tanh function. The limit point (which cause multiple steady-state solutions from a singular point) are very beneficial because it enables the Multiobjective nonlinear model predictive control calculations to converge to the Utopia point (the best possible solution) in the model.

Keywords: Bifurcation; Optimization; Control; Damkohler Number

Background

Verazaluce-García, et al.[1], investigated the steady-state nonlinear bifurcation analysis of a high-impact polystyrene continuous stirred tank reactor. Zukowski, et al.[2] studied the generation of chaotic oscillations in a system with flow reversal. Antonelli, et al. investigated the stabilization of continuous stirred tank reactors. Merta[4] determined the characteristic time series and operation region of the system of two tank reactors (CSTR) with variable division of recirculation stream. Berezowski, et al.[5] studied the periodicity of chaotic solutions of the model of thermally coupled cascades of chemical tank reactors with flow reversal. Berezowski[6] investigated the application of the parametric continuation method for determining steady state diagrams in chemical engineering. Berezowski[7] studied limit cycles that do not comprise steady states of chemical reactors. Berezowski[8], Determination of Hopf bifurcation sets of a chemical reactors by a two-parameter continuation method. In this work, bifurcation analysis and multiobjective nonlinear model predictive control is performed on a chemical reactor model[8]. 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 presented, followed by the conclusions.

Model Equations[8]

The model equations are

$$\phi = da*(1-\alpha)^n exp(\frac{\gamma\beta\theta}{1+\beta\theta})$$

$$\frac{d(\alpha)}{dt} = -\alpha + \phi$$

$$\frac{d(\theta)}{dt} = \frac{(delta*(\theta h - \theta) + \phi - \theta)}{Le}$$

$\alpha, \theta, \theta h; da; Le$ are the degree of conversion, dimensionless temperature, dimensionless temperature of cooling system, Damkohler number and Lewis number. The base parameter values are $\gamma = 15;\ \beta = 2;\ \delta = 1.5;\ n = 1.5;\ \mathrm{Le} = 1;\ da = 0.03;\ \theta h = 0.165$. $\theta h; da$ are the bifurcation parameters and control variables.

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[9,10]. This program detects Limit points (LP), branch points (BP), and Hopf bifurcation points(H) for an ODE system

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

$x \in R^n$ 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

$$Aw = 0$$

Where A is

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

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

$y = (y_1, y_2, y_3, y_4, ...y_n)$ must align with $\hat{w} = (w_1, w_2, w_3, w_4, ...w_n)$. Since

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

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

$$Az = 0$$

$$Aw = 0$$

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,

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

$@$ 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[11-13].

Hopf bifurcations cause limit cycles. The tanh activation function (where a control value u is replaced by) $(u \tanh u / \varepsilon)$ is used to eliminate spikes in the optimal control profiles[14-17]. Sridhar[18] explained with several examples how the activation factor involving the tanh function also eliminates the Hopf bifurcation points. This was because the tanh function increases the oscillation time period in the limit cycle.

Multiobjective Nonlinear Model Predictive Control(MNLMPC)

The rigorous multiobjective nonlinear model predictive control (MNLMPC) method developed by Flores Tlacuahuaz, et al.[19] 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

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

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 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 multiobjective optimal control (MOOC) problem that will be solved is

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

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

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[20] 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[21] and confirmed as a global solution with BARON[22].

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 $\sum_{t_i=0}^{t_i=t_f} q_j(t_i) = q_j^*$ for all j.

Sridhar[23] demonstrated that when the bifurcation analysis revealed the presence of limit and branch points the MNLMPC calculations to converge to the Utopia solution . For this, the singularity condition, caused by the presence of the limit or branch points was imposed on the co-state equation[24]. 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

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

Differentiating the objective function results in

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

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

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

The optimal control co-state equation

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

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

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

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 optimal solution is the Utopia solution.

Results and Discussion

When da was used as the bifurcation parameter, two limit points and one Hopf bifurcation points were observed (α, θ, da) values of (0.231511 0.191604 0.005387), (0.448434 0.278374 0.005123 and (0.683158 0.372263 0.006354) **(Figure 1a)**. When da is modified to da(tanh(da))/5000; the Hopf bifurcation disappears **(Figures 1b and 1c)**.

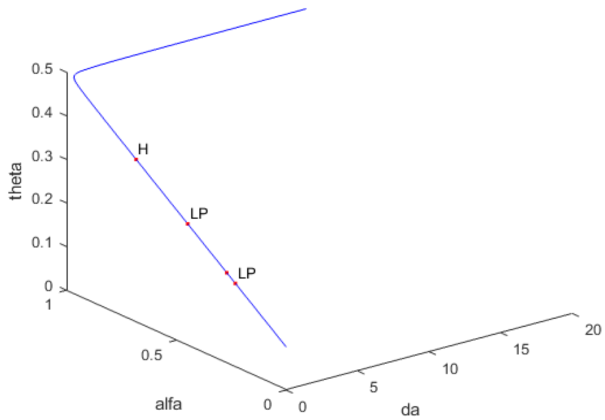

Figure 1a: Bifurcation Diagram when da is the bifurcation parameter.

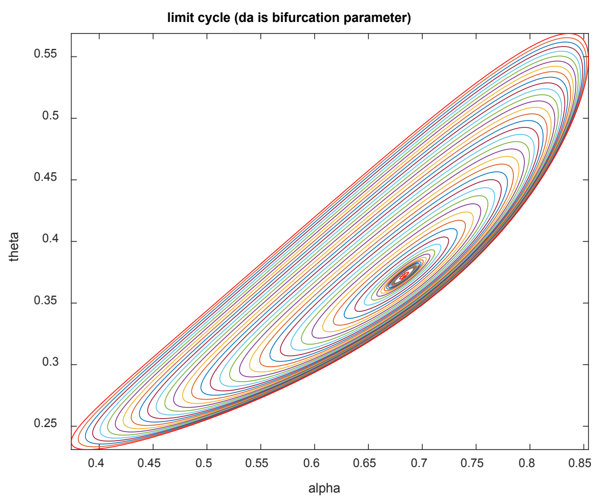

Figure 1b: Limit cycle when da is the bifurcation parameter.

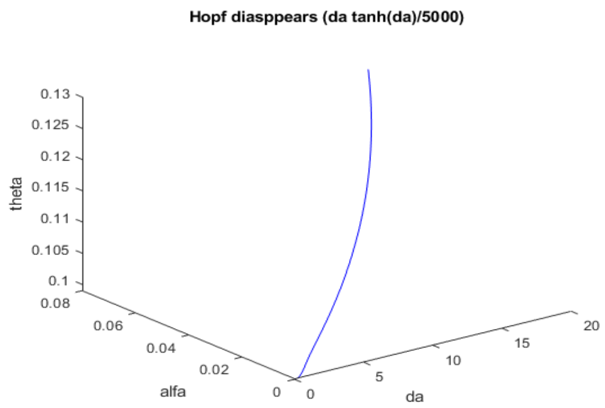

Figure 1c: Hopf disappears when da is modified to da(tanh(da))/5000.

When θh was used as the bifurcation parameter, two limit points and one Hopf bifurcation points were observed $(\alpha, \theta, \theta h)$ values of (0.128807 0.062386 0.018105) (0.643032 0.221859 -0.058923), (0.793557 0.301447 -0.026626). **(Figure 1d)**. The limit cycle caused by this Hopf bifurcation is shown in **(Figure 1e)** When θh was modified to $\theta h \tanh(\theta h)$

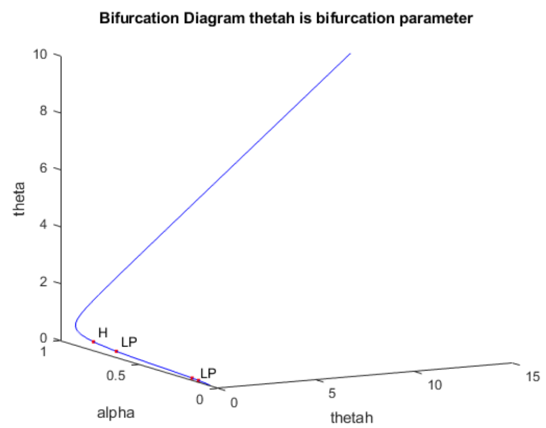

Figure 1d: Bifurcation Diagram when θh is the bifurcation parameter.

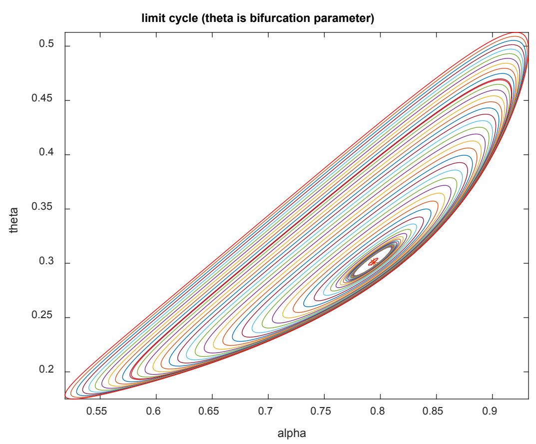

Figure 1e: limit cycle when θh is the bifurcation parameter.

A close curve was detected with 2 limit points at (0.128807 0.062386 0.134961) and (0.128807 0.062386 -0.13496). The Hopf bifurcation point disappears **(Figure 1f)**.

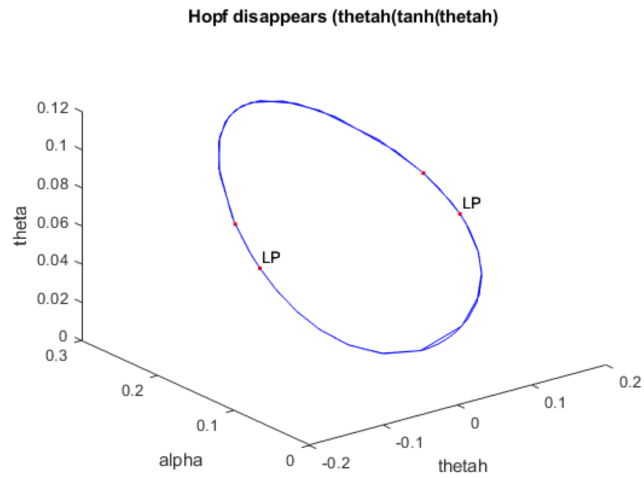

Figure 1f: Hopf disappears when θh is modified to $\theta h(\tanh(\theta h))$.

In both cases, the use of the tanh activation factor eliminated the limit cycle causing Hopf bifurcation, validating the analysis in Sridhar[18]

For the MNLMPC calculations in the model , $\sum_{t_{i=0}}^{t_i=t_f} \alpha(t_i)$ was maximized , and $\sum_{t_{i=0}}^{t_i=t_f} \theta h(t_i)$ was minimized leading to values of 1.99911320507 and 0. The overall optimal control problem will involve the minimization of $(\sum_{t_{i=0}}^{t_i=t_f} \alpha(t_i) - 1.99911320507)^2 + (\sum_{t_{i=0}}^{t_i=t_f} \theta h(t_i) - 0)^2$ was minimized subject to the equations governing the model. This led to a value of zero the Utopia.

The MNLMPC values of the control variables, $\theta h; da$ were 0.1786 and 0.2613. The various MNMPC figures are shown in **(Figures 2a-2d)**. The presence of the limit and branch points is beneficial because it allows the MNLMPC calculations to attain the Utopia solution, validating the analysis of Sridhar[23].

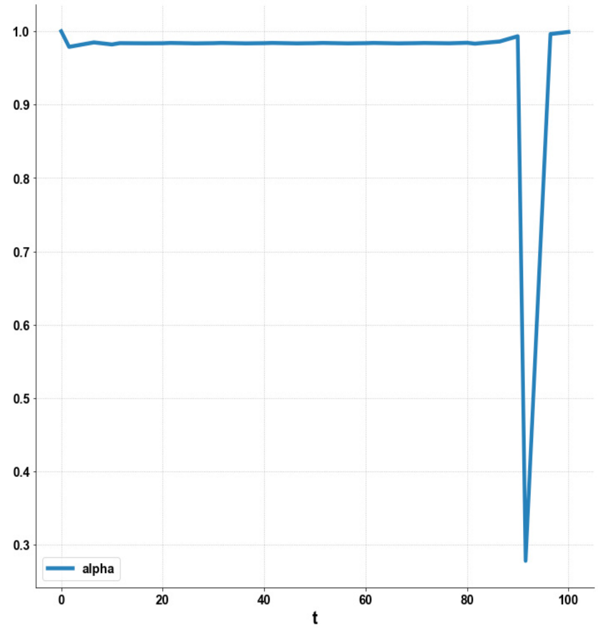

Figure 2a: MNLMNC α vs t.

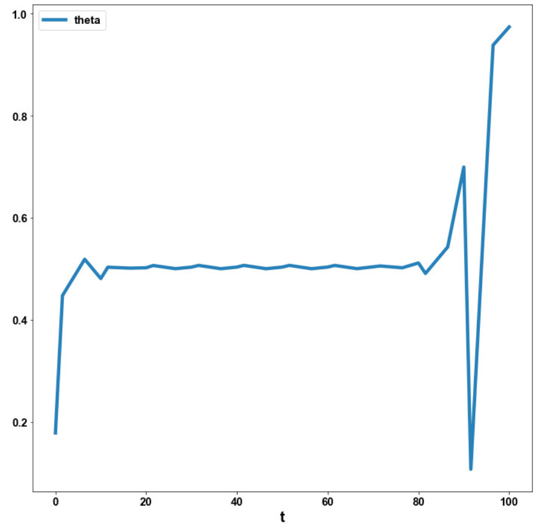

Figure 2b: MNLMC θ vs t.

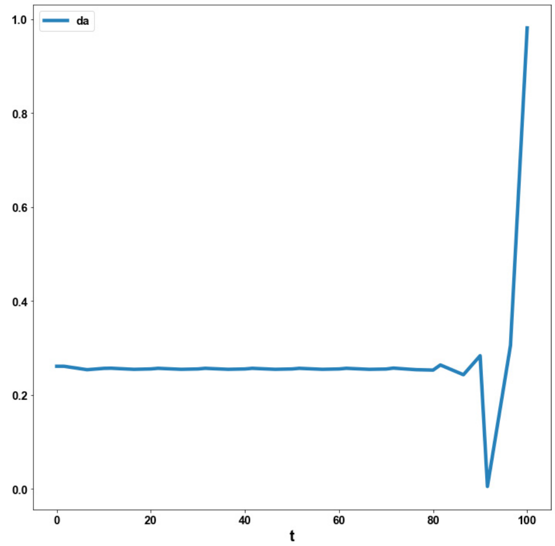

Figure 2c: MNLMC θ vs t.

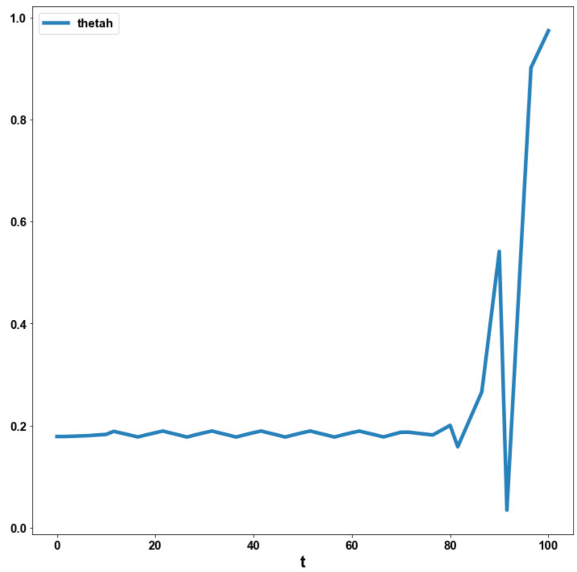

Figure 2d: MNLMC θh vs t.

Conclusions

Bifurcation analysis and multiobjective nonlinear control (MNLMPC) studies on a chemical reactor dynamic model. The bifurcation analysis revealed the existence of Hopf bifurcation points and limit points The Hopf bifurcation point, which causes an unwanted limit cycle, is eliminated using an activation factor involving the tanh function. The 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 models. A combination of bifurcation analysis and Multiobjective Nonlinear Model Predictive Control(MNLMPC) for the Lorenz-84 atmospheric circulation model 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.

Acknowledgement

Dr. Sridhar thanks Dr. Carlos Ramirez and Dr. Suleiman for encouraging him to write single-author papers

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