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Reduced-Order Modeling, Hopf Bifurcation, and Bifurcation-Aware Optimal Control in Nonlinear Reacting Fluid Systems

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ABSTRACT

Oscillatory instabilities arising from the nonlinear interaction of reaction and transport processes can significantly degrade the performance, stability, and safety of reacting fluid systems. Reduced-order models provide an efficient framework for capturing the essential nonlinear dynamics while enabling systematic bifurcation analysis and optimal control design. A nonlinear reduced-order framework is developed by projecting the governing partial differential equations describing coupled momentum and scalar transport onto a low-dimensional modal basis, resulting in a four-dimensional dynamical system with two velocity modes and two reactive scalar modes. Stability and bifurcation analyses are performed using MATCONT to identify Hopf bifurcation points and limit cycle dynamics. An optimal control problem is subsequently formulated in Pyomo.DAE and solved using IPOPT to minimize oscillatory energy while incorporating a bifurcation-aware constraint that prevents operation near the Hopf boundary. The bifurcation analysis identifies a Hopf bifurcation at a critical Damköhler number, where a complex conjugate pair of eigenvalues crosses the imaginary axis. The optimal control results demonstrate that incorporating the Hopf bifurcation avoidance constraint suppresses oscillatory dynamics, achieving approximately a 90% reduction in the objective function compared with the unconstrained formulation. The proposed reduced-order modeling and control framework provides a low-dimensional, physically motivated representation for investigating oscillatory instabilities in reacting fluid systems. Integrating bifurcation analysis with optimal control provides a computational strategy for maintaining stable operation and suppressing self-sustained oscillations. The present model is intended as a conceptual proof-of-principle framework; validation against full-resolution simulations or experimental reacting-flow data remains an important direction for future work.

1. Introduction

Reacting fluid systems exhibit a wide range of nonlinear dynamical behaviors arising from the coupled interaction between advection, diffusion, and chemical reaction processes. These interactions are fundamental to many engineering and natural systems, including combustion chambers, catalytic reactors, environmental flows, and geophysical transport processes. A key feature of such systems is the emergence of self-sustained oscillations and instability-driven transitions, which are often associated with complex feedback mechanisms between velocity fields and scalar quantities such as temperature or species concentration. Understanding and controlling these behaviors remains a central challenge in nonlinear fluid mechanics and reactive transport theory.

From a physical perspective, reacting flows are governed by coupled partial differential equations describing momentum balance and scalar transport. The nonlinear advection term introduces mode coupling within the velocity field, while reaction kinetics introduce nonlinear source terms that can amplify or damp scalar fluctuations depending on the local state of the system. In addition, diffusion processes act to smooth gradients, providing a stabilizing influence. The competition between these



mechanisms often leads to rich dynamical regimes, including steady states, oscillatory solutions, and chaotic behavior. In particular, oscillatory instabilities arising through Hopf bifurcation mechanisms are frequently observed in chemically reacting systems and thermo-fluid applications.

Despite the high dimensionality of the governing equations, many essential features of reacting flow dynamics can be captured using reduced-order models. Such models are typically constructed using modal decomposition techniques, where the full field variables are projected onto a small number of dominant spatial modes. This approach yields a finite-dimensional system of ordinary differential equations governing the temporal evolution of modal amplitudes. Reduced-order modeling not only simplifies the mathematical structure of the problem but also provides physical insight into dominant instability mechanisms and energy transfer pathways between modes.

In the present work, a four-dimensional reduced-order model is developed to describe the coupled dynamics of a reacting fluid system. The model consists of two velocity modes and two scalar modes, representing the dominant energetic structures in the flow and reactive field, respectively. Linear terms in the model represent viscous dissipation and diffusive decay, while nonlinear terms capture convective interactions and mode coupling effects. The scalar field is further governed by a cubic reaction law, which introduces nonlinear saturation and represents the balance between growth induced by reaction kinetics and self-limiting effects at higher amplitudes. The coupling between velocity and scalar fields provides a feedback mechanism through which chemical activity influences fluid motion and vice versa.

A distinctive feature of the proposed model is the inclusion of a rotational coupling structure in the velocity subspace. This skew-symmetric interaction introduces oscillatory dynamics into the linearized system and enables the emergence of complex conjugate eigenvalues. As a result, the system is capable of exhibiting Hopf bifurcation behavior under variation of key parameters. In this study, the Damköhler number is identified as the principal bifurcation parameter, representing the ratio between reaction and transport time scales. Changes in this parameter alter the balance between nonlinear growth and dissipative mechanisms, thereby controlling the onset of oscillatory instability.

To analyze the stability structure of the system, numerical continuation techniques are employed using MATCONT. This allows for systematic tracking of equilibrium branches and identification of bifurcation points in parameter space. The analysis reveals the presence of a Hopf bifurcation at a critical parameter value, where a pair of complex conjugate eigenvalues crosses the imaginary axis. The associated first Lyapunov coefficient indicates the nature of the bifurcation and the stability of the emerging limit cycles. These results confirm that the reduced-order model captures essential nonlinear mechanisms responsible for oscillatory behavior in reacting fluid systems.

In addition to bifurcation analysis, this work investigates the suppression and regulation of oscillatory dynamics through optimal control. A dynamic optimization framework is formulated using Pyomo.DAE and solved using IPOPT. The objective function is designed to minimize oscillatory energy in the modal amplitudes while accounting for control effort. Furthermore, a bifurcation-aware constraint is introduced to prevent the system from operating near the Hopf instability boundary. This approach enables proactive stabilization by steering the system away from parameter regimes where oscillatory behavior is likely to emerge.

The combination of reduced-order modeling, bifurcation analysis, and optimal control provides a unified framework for understanding and managing nonlinear dynamics in reacting fluid systems. The results demonstrate that explicit incorporation of instability structure into the control formulation significantly enhances performance compared to conventional energy-based optimization strategies. This suggests a promising direction for the development of stability-informed control methodologies for complex nonlinear distributed systems.

Overall, the present study contributes to the development of physically interpretable reduced-order models for reacting flows and establishes a computational framework for analyzing and controlling oscillatory instabilities. The methodology provides a bridge between dynamical systems theory and chemical engineering applications, with potential relevance to combustion control, reactive transport processes, and environmental fluid systems.

The theoretical foundations of scalar transport in fluid flows were established through early studies on dispersion in laminar and turbulent regimes, where analytical descriptions of solute spreading in moving fluids were developed and formalized in classical transport theory [1], [2]. These works provided the first rigorous framework for understanding how advective motion couples with molecular diffusion to determine macroscopic transport behavior in fluids. Building on these ideas, the development of combustion theory and reacting flow physics introduced the role of chemical source terms in modifying transport dynamics, particularly through the introduction of characteristic reaction–transport scaling concepts [3-5].

Subsequent advances in turbulence theory and combustion modeling emphasized the importance of multiscale interactions between velocity fluctuations and scalar fields, leading to refined descriptions of energy cascades and scalar dissipation in turbulent flows [6-8]. These studies highlighted that reacting flows cannot be treated as simple passive transport systems, as chemical reactions actively modify flow structure and vice versa [9]. This led to the development of foundational combustion frameworks that integrate fluid mechanics, chemical kinetics, and diffusion processes into unified modeling approaches [10], [11].

During the 2000s, significant progress was made in turbulent combustion modeling, particularly through the introduction of flamelet concepts, probability density function methods, and large-eddy simulation approaches for reacting flows [12-14]. These frameworks enabled more accurate representation of turbulence-chemistry interaction while maintaining computational tractability in high-dimensional systems. In parallel, detailed analyses of flame stability and structure demonstrated how scalar gradients and reaction zones govern flame propagation and extinction phenomena [15-17].

Direct numerical simulations of reacting flows further advanced understanding of flame–turbulence interaction by resolving all relevant spatial and temporal scales, revealing detailed mechanisms of scalar mixing, reaction front evolution, and localized extinction events [18-20]. These studies confirmed that nonlinear coupling between advection, diffusion, and reaction terms plays a central role in determining flow stability and combustion efficiency.

More recent developments have focused on improving physical modeling of multiphase reacting flows and scalar transport in complex geometries, where additional interactions such as particle loading, compressibility effects, and Lagrangian mixing processes become important [21], [22]. High-fidelity computational studies have also provided detailed insights into reaction zone structure and turbulence–chemistry coupling mechanisms in canonical and industrial flow configurations [23-25].

Finally, modern research continues to refine closure models for multi-component reacting systems, emphasizing improved representation of unresolved scales and more accurate coupling between chemical kinetics and turbulent transport processes [26-28]. These developments collectively form the foundation for contemporary reduced-order modeling approaches, where the goal is to retain essential nonlinear physics in low-dimensional systems suitable for analysis, control, and bifurcation studies.

Reduced-order modeling has increasingly been used to obtain computationally tractable representations of complex fluid dynamical systems. Projection-based approaches, including proper orthogonal decomposition and Galerkin projection, enable high-dimensional governing equations to be represented by a smaller number of dominant dynamical variables while retaining the principal structures required for analysis and control [29], [30]. Rowley and Dawson reviewed reduced-order

approaches for fluid-flow analysis and control, emphasizing the role of low-dimensional representations in extracting dominant flow physics and facilitating control design [29]. Benner et al. similarly demonstrated the importance of projection-based model reduction for parameter-dependent dynamical systems, where repeated analysis over varying operating parameters would otherwise be computationally expensive [30].

Reduced-order models are particularly useful for studying nonlinear stability and bifurcation phenomena because equilibrium branches, eigenvalue variations, and periodic solutions can be investigated efficiently within a low-dimensional state space. Recent work demonstrated that reduced-order models can reproduce important features associated with Hopf bifurcations in fluid systems, including precritical equilibria, the bifurcation point, and postcritical limit-cycle oscillations [31]. Such studies illustrate the importance of constructing reduced models that retain the nonlinear dynamical structures responsible for transitions between steady and oscillatory regimes.

Reduced-order modeling also provides an attractive framework for control and optimization because the reduced computational cost permits repeated evaluation of nonlinear system dynamics during optimization. In particular, reduced models can connect the dominant dynamical states with control variables while avoiding the computational expense associated with repeatedly solving the complete distributed-parameter system. Consequently, combining reduced-order dynamics with bifurcation information provides a potential strategy for designing controls that account explicitly for changes in system stability rather than relying exclusively on conventional state- or energy-based objectives [29].

Despite these developments, comparatively less attention has been directed toward integrating reduced-order reaction-transport modeling, numerical continuation, Hopf-bifurcation characterization, machine-learning-based stability approximation, and bifurcation-aware dynamic optimization within a single computational framework. The present work addresses this methodological gap using a physically motivated four-dimensional nonlinear model as a conceptual test system. The objective is not to reproduce the full complexity of a specific turbulent combustion configuration, but rather to investigate how nonlinear reaction-transport coupling, bifurcation analysis, stability prediction, and optimal control can be combined within a computationally tractable low-dimensional framework.

The primary objective of this research is to develop a mathematically consistent and computationally tractable reduced-order framework for analyzing nonlinear oscillatory behavior in reacting fluid systems, with particular emphasis on Hopf bifurcation phenomena and their control. The study seeks to bridge dynamical systems theory, fluid mechanics, and optimal control in order to provide both physical insight and practical tools for managing instability-driven behavior in chemically reacting flows.

A first objective is to construct a physically motivated reduced-order model that captures the essential interaction mechanisms between fluid motion and reactive scalar transport. This includes the representation of viscous dissipation, nonlinear convection, scalar-flow coupling, and nonlinear reaction kinetics within a low-dimensional modal structure. The model is designed to retain only the dominant dynamical features necessary for the emergence of oscillatory instabilities while remaining sufficiently simple for analytical and numerical bifurcation analysis.

A second objective is to systematically investigate the stability structure of the resulting dynamical system using numerical continuation methods. In particular, the study aims to identify Hopf bifurcation points, characterize their nature through computation of Lyapunov coefficients, and analyze the transition from steady-state to oscillatory regimes. This provides a rigorous understanding of how variations in the Damköhler number and coupling parameters influence the onset of self-sustained oscillations.

A third objective is to validate the existence of limit cycle behavior associated with the Hopf bifurcation through direct numerical simulation and continuation results. This includes confirming the eigenvalue structure at the critical point and examining the amplitude and qualitative structure of periodic solutions in the post-bifurcation regime.

A fourth objective is to develop an optimal control framework based on Pyomo.DAE that minimizes oscillatory energy in the system while accounting for nonlinear dynamical constraints. The formulation incorporates both state-dependent performance measures and control effort penalties, enabling systematic suppression of undesired oscillatory behavior.

A fifth objective is to introduce and evaluate a bifurcation-aware control strategy that explicitly incorporates Hopf instability information into the optimization problem. This includes enforcing constraints that prevent operation near critical bifurcation boundaries and assessing the resulting improvement in performance relative to unconstrained control formulations.

Finally, the research aims to demonstrate the broader applicability of the proposed framework to nonlinear reacting flow systems where stability, efficiency, and control are critical. The overarching goal is to establish a general methodology for combining reduced-order modeling, bifurcation analysis, and optimal control for complex nonlinear dynamical systems exhibiting oscillatory instabilities.

The novelty of this research lies in the development of a unified reduced-order and control framework that explicitly integrates nonlinear fluid-reaction interactions, Hopf bifurcation structure, and optimal control design within a single mathematically consistent formulation. While reduced-order modeling and bifurcation analysis have been widely studied in fluid mechanics and chemical reaction systems separately, the present work combines these elements in a way that enables both mechanistic interpretation and direct control of oscillatory instabilities.

A key novel aspect is the construction of a four-dimensional coupled oscillator model that simultaneously captures velocity-velocity nonlinear interactions, velocity-scalar coupling, scalar advection effects, and cubic reaction kinetics. This structure is sufficiently rich to generate Hopf bifurcations while remaining low-dimensional enough for systematic analytical treatment and numerical continuation. The model provides a minimal yet physically interpretable representation of reacting flow instability mechanisms.

Another important contribution is the explicit identification and characterization of Hopf bifurcation behavior in the reduced system using MATCONT, including computation of equilibrium branches, detection of critical parameter values, and evaluation of the first Lyapunov coefficient. The ability to recover both the bifurcation point and the associated limit cycle dynamics within a controlled reduced-order setting demonstrates that the proposed formulation preserves essential nonlinear stability features of the underlying physical system.

A further novelty is the integration of bifurcation information directly into an optimal control framework formulated in Pyomo.DAE and solved using IPOPT. Unlike traditional optimal control approaches that minimize energy or tracking error alone, the present methodology incorporates an instability-aware structure by penalizing oscillatory energy and constraining trajectories relative to the Hopf bifurcation boundary. This represents a shift from reactive control strategies to bifurcation-informed predictive control design.

In addition, the study introduces a comparative analysis between unconstrained and bifurcation-constrained optimal control formulations, demonstrating quantitatively that explicit consideration of Hopf structure leads to substantial performance improvement. The observed reduction in the objective function highlights the effectiveness of embedding dynamical systems information into the optimization problem.

Overall, the research is novel in its coupling of reduced-order reacting flow modeling, rigorous bifurcation analysis, and stability-aware optimal control within a single computational pipeline. This integrated approach provides a new pathway for analyzing, predicting, and controlling nonlinear oscillatory behavior in complex reacting fluid systems.

The rest of this paper is organized as follows. First, the model equations are presented, followed by a description of the numerical procedures used. The results discussion and conclusions are then presented.

2. Research and Methodology

The present study considers a simplified representation of reacting fluid dynamics in which nonlinear interactions between hydrodynamic modes and chemical reaction kinetics give rise to oscillatory instabilities. The motivation for this formulation stems from the observation that many reacting flow systems, particularly those involving exothermic reactions or strongly coupled transport–reaction processes, exhibit self-sustained oscillations, amplitude modulation, and bifurcation phenomena that cannot be captured by purely linear models.

In high-dimensional fluid systems, such dynamics arise from the coupling between advective transport, viscous dissipation, and nonlinear reaction source terms. However, direct numerical simulation of the full governing partial differential equations is often computationally expensive and analytically intractable for the purpose of bifurcation analysis and control design. To address this, reduced-order modeling techniques are employed to extract the dominant dynamical behavior of the system in a low-dimensional state space.

In the present formulation, it is assumed that the flow field and scalar (reacting species or temperature) field can be accurately represented using a small number of dominant spatial modes. These modes may be interpreted as energetic structures obtained from Galerkin projection, proper orthogonal decomposition, or other modal decomposition techniques. The temporal evolution of the system is then governed by the amplitudes of these modes, which evolve according to nonlinear ordinary differential equations.

The resulting reduced-order system retains the essential physical mechanisms responsible for instability. Linear terms represent viscous dissipation in the velocity field and diffusive-reactive decay in the scalar field. Nonlinear terms arise from convective transport and mode-mode interactions, which redistribute energy between dominant structures. In addition, coupling terms between the scalar and velocity modes represent feedback mechanisms whereby reaction-induced density or temperature variations influence the flow field, and conversely, advective transport modifies the spatial distribution of the reactive scalar.

A key feature of the model is the inclusion of a cubic nonlinear reaction law, which captures saturation effects commonly observed in chemical kinetics. This term prevents unbounded growth of the scalar modes and introduces nonlinear damping at large amplitudes. The balance between linear growth induced by reaction kinetics and nonlinear saturation plays a central role in determining the stability of steady states.

To capture oscillatory behavior observed in reacting flow systems, a rotational coupling between velocity modes is introduced. This structure generates a skew-symmetric contribution in the linearized dynamics, leading to complex-conjugate eigenvalues and enabling Hopf bifurcation phenomena. As a result, the reduced-order system is capable of exhibiting transitions from steady-state behavior to stable or unstable limit cycles depending on the system parameters.

Within this framework, the Damköhler number is identified as the primary bifurcation parameter, representing the relative strength of chemical reaction rates compared to transport processes.

Variation of this parameter alters the balance between growth and dissipation mechanisms, thereby governing the onset of oscillatory instability. The resulting low-dimensional system provides a tractable yet physically interpretable model for studying bifurcation structure, nonlinear dynamics, and potential control strategies in reacting fluid flows. We consider an incompressible reacting flow with a scalar concentration (or temperature) field. The governing equations are

$$\begin{aligned}\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} &= -\nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{F}(c) \\ \frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c &= D \nabla^2 c + R(c)\end{aligned}\quad (1)$$

where $\mathbf{u}$ is the velocity field, c is the scalar field, $R(c)$ is the reaction source term, and $\mathbf{F}(c)$ represents feedback of the scalar on the flow. To obtain a reduced-order representation, we assume that the dynamics are dominated by two velocity modes and two scalar modes. The velocity and scalar fields are expanded as:

$$\begin{aligned}\mathbf{u}(x, t) &= a_1(t) \phi_1(x) + a_2(t) \phi_2(x) \\ c(x, t) &= b_1(t) \psi_1(x) + b_2(t) \psi_2(x)\end{aligned}\quad (2)$$

where a_1, a_2, b_1, b_2 are time-dependent modal amplitudes. Applying Galerkin projection onto the corresponding basis functions yields a set of ordinary differential equations governing the evolution of the modal amplitudes. The viscous and diffusive terms contribute linear damping in each mode, $\sigma_1 a_1, \sigma_2 a_2, \gamma_1 b_1, \gamma_2 b_2$. The nonlinear convective term $(\mathbf{u} \cdot \nabla) \mathbf{u}$ generates quadratic interactions between velocity modes, which are retained in the form $c_1 a_1 a_2, c_2 a_1 a_2$.

The coupling from the scalar field back to the velocity field arises through projection of $\mathbf{F}(c)$, giving $\beta_1 b_1, \beta_2 b_2$. Similarly, the advection of the scalar field by the velocity field produces velocity-scalar interaction terms of the form $c_3 a_1 b_1, c_4 a_2 b_2$. The reaction kinetics are modeled using a cubic nonlinear law

$$R(b) = Dab - b^3 \quad (3)$$

where Da is the Damköhler number, defined as the ratio of reaction rate to transport rate. To allow for the oscillatory dynamics, a rotational coupling between velocity modes is introduced in the form $-\omega a_2 + \omega a_1$. Combining all contributions, the final reduced-order model is:

$$\begin{aligned}\frac{da_1}{dt} &= \sigma_1 a_1 - \omega a_2 + \beta_1 b_1 + c_1 a_1 a_2 \\ \frac{da_2}{dt} &= \omega a_1 + \sigma_2 a_2 + \beta_2 b_2 + c_2 a_1 a_2 \\ \frac{db_1}{dt} &= \gamma_1 b_1 + c_3 a_1 b_1 + Dab_1 - b_1^3 \\ \frac{db_2}{dt} &= \gamma_2 b_2 + c_4 a_2 b_2 + Dab_2 - b_2^3\end{aligned}\quad (4)$$

Tables 1 and 2 provide details about the variables and parameters contained in the appendix.

3. Numerical Methods

3.1. Bifurcation Analysis

Continuation and bifurcation computations were carried out using the MATLAB-based software MATCONT. Bifurcation analysis provides important insights into the mechanisms underlying the existence of multiple steady states and self-sustained oscillations in nonlinear dynamical systems. In particular, branch points and limit points are associated with the emergence of multiple steady-state solutions, whereas oscillatory dynamics and periodic solutions originate from Hopf bifurcations. The package, originally developed and subsequently enhanced by several researchers, enables the systematic identification of limit points (LP), branch points (BP), and Hopf bifurcation points (H) in nonlinear dynamical models [30]. This program identifies Limit points (LP), branch points (BP), and Hopf bifurcation points (H) for an system of ordinary differential equations

$$\frac{dx}{dt} = f(x, \alpha) \quad (5)$$

$x \in R^n$ where the bifurcation parameter is α .

At a limit point, the $n+1^{th}$ component of the tangent vector $w_{n+1} = 0$. For a branch point,

the matrix $B = \begin{bmatrix} A \\ w^T \end{bmatrix}$ must be singular and have a determinant of 0.

At a Hopf bifurcation point,

$$\det(2f_x(x, \alpha) @ I_n) = 0 \quad (6)$$

@ indicates the bilateral product while I_n is the n-square identity matrix. More details can be found in Kuznetsov and Govaerts, respectively [31], [32].

3.2. Optimal Control

Pyomo.dae is used for the Optimal Control calculations. Pyomo with its Pyomo.DAE module provides an efficient framework for the formulation and solution of dynamic optimization problems involving systems of differential and algebraic equations [33]. The package provides a symbolic modeling environment for representing differential-algebraic equation (DAE) systems in optimization applications. In Pyomo.DAE, the continuous-time dynamic model, is transformed into a nonlinear programming (NLP) problem through discretization techniques such as orthogonal collocation, allowing the resulting optimization problem to be solved using standard NLP solvers. The NLP is solved using IPOPT [34].

3.3. Construction of the Stability Dataset Using MATCONT Results

A stability dataset was constructed using the numerical continuation results generated in MATCONT. Each entry in the dataset corresponds to a continuation point along an equilibrium branch. For every point, the recorded information includes the state variables, the bifurcation parameter, and a numerical indicator of stability.

The stability indicator was obtained from the Jacobian matrix evaluated numerically at each equilibrium point. MATLAB was then used to calculate the eigenvalues of the Jacobian, after which the

largest real component among all eigenvalues was selected as the stability metric. This value was computed using the MATLAB command `eig_real_max = max(real(eigvals))`.

This scalar metric provides a quantitative characterization of the local stability of an equilibrium. A negative value indicates that the equilibrium is locally asymptotically stable, whereas a positive value signifies instability. A transition of the metric through zero is associated with the occurrence of a Hopf bifurcation. After all continuation points were processed, the resulting stability dataset was exported in CSV format. The generated dataset can subsequently serve as input for computational analyses, including classification and regression models, to identify stability boundaries and approximate bifurcation locations.

3.4. Development of a Neural Network Surrogate Model for Stability Prediction

Directly incorporating eigenvalue computations into an IPOPT-based optimal control framework is generally impractical for several reasons. First, evaluating eigenvalues at every optimization time step introduces a substantial computational burden. Second, the relationship between the system states and the maximum real eigenvalue becomes non-smooth near eigenvalue crossings, making gradient-based optimization more difficult. Third, obtaining symbolic derivatives of eigenvalues is mathematically complex and computationally demanding.

Prior to training the neural network, all input features were standardized to improve numerical conditioning and enhance the convergence and stability of the learning process. Let X_{raw} represent the vector of state variables and bifurcation parameters extracted from the stability dataset. For each input variable (j), the mean μ and standard deviation σ_j were determined from all samples in the training dataset. The mean of the (j) input variable was calculated as the arithmetic average of the corresponding training samples and is expressed as:

$$\mu_j = \frac{1}{N} \sum_{k=1}^N x_j^{(k)}$$

and the training standard deviation for the input variable j is defined as:

$$\sigma_j = \frac{1}{N} \left(\sum_{k=1}^N x_j^{(k)} - \mu_j \right)^2 \quad (7)$$

The standardized inputs were defined as

$$x_j = \frac{x_{raw,j} - \mu_j}{\max(\sigma_j, \epsilon_{scale})} \quad (8)$$

where ϵ_{scale} is a small positive regularization constant introduced to avoid numerical instability caused by input variables with extremely low variance. This adjustment maintains an appropriate scaling of all input features while preventing excessively large activation values within the neural network during optimization. As a result, the normalization process improves the numerical conditioning of the neural network and increases the reliability of gradient-based optimization algorithms.

The normalization parameters, namely the training mean (μ), (σ), and standard deviation (μ), (σ), were saved after training and incorporated directly into the Pyomo optimal control model. Using the same normalization parameters during both training and deployment ensures that the neural network receives consistently scaled inputs throughout the optimization procedure.

To eliminate the need for repeated eigenvalue evaluations during optimization, a feedforward neural network was developed to approximate the maximum real eigenvalue as a smooth function of the system states and the bifurcation parameter. This surrogate model replaces the computationally intensive eigenvalue calculations while preserving the smoothness required by gradient-based solvers. Hyperbolic tangent (Tanh) activation functions were selected because they are continuously differentiable, making them well-suited for integration with IPOPT.

Let (x) denote the vector of normalized input variables. The feedforward neural network can then be expressed as

$$\begin{aligned} z_1 &= \tanh(W_1 x + b_1) \\ z_2 &= \tanh(W_2 z_1 + b_2) \\ \lambda_{\max_NN} &= W_3 z_2 + b_3 \end{aligned} \quad (9)$$

Where W_i and b_i denote the weight matrices and bias vectors, respectively. The hidden-layer variables z_1 and z_2 represent nonlinear transformations of the input variables and intermediate features. The final output $\hat{\lambda}_{\max}$ provides a smooth approximation of the spectral abscissa. Because tanh is infinitely differentiable, the network is fully smooth, guaranteeing the availability of first and second derivatives required by IPOPT. Without biases, the network output would be constrained to pass through the origin, limiting flexibility.

The hidden-layer outputs, denoted by z_1 and z_2 , capture nonlinear transformations of the input variables and the features generated by the preceding layer, respectively. Specifically, each component of z_1 represents a smooth nonlinear combination of the normalized input variables, whereas each component of z_2 corresponds to a higher-level feature obtained by further processing the representations learned in z_1 . The final output $\lambda_{\max_NN}$ provides a smooth approximation of the maximum real eigenvalue, enabling efficient and differentiable stability evaluation within the optimal control problem. The surrogate model is incorporated into the optimal control formulation through a soft-penalty approach. In this framework, a smooth_max function is employed to transform the predicted maximum real eigenvalue, λ , into a smooth, non-negative penalty term. This penalty remains negligible when the system is stable and increases continuously as the predicted eigenvalue becomes positive, thereby activating only when unstable operating conditions are approached.

$$s_{\max}(\lambda + \varepsilon_1) = \text{smooth} - \max(\lambda + \varepsilon_1) = \frac{(\lambda + \varepsilon_1) + \sqrt{(\lambda + \varepsilon_1)^2 + \varepsilon_1}}{2} \quad (10)$$

λ is the neural network's predicted maximum eigenvalue at the current state and parameter, while ε is a small positive safety margin to ensure differentiability. The soft penalty formulation involves the new objective function, where the original objective function $\sum \text{optv}(t) = \sum (a_1(t))^2 + (a_2(t))^2 + (Da(t))^2$ is modified to $\sum (\text{optv}(t) + \alpha_{\text{hopf}} \cdot s_{\max}(\lambda + \varepsilon_1))^2$. α_{Hopf} controls how aggressively instability is penalized, and prevents numerical issues at exactly $\lambda = 0$ and slightly shifts the stability boundary. When α_{Hopf} is 0, no Hopf constraint is implemented. The goal is to minimize the objective function value while ensuring differentiability for IPOPT and avoiding non-smoothness in the optimization. The objective function used minimizes oscillatory energy and control effort. This formulation eliminates the need for repeated eigenvalue evaluations while providing a smooth and continuously differentiable approximation that is well suited for gradient-based optimization methods. Consequently, stability considerations can be incorporated directly into the

optimal control problem through the surrogate model, avoiding explicit eigenvalue calculations throughout the optimization process.

To enable seamless integration with the optimal control framework, a stability dataset was generated from the continuation results obtained using MATCONT. For each equilibrium point along the continuation branch, the Jacobian matrix was evaluated numerically, and the corresponding eigenvalues were subsequently calculated. The stability metric is defined as the largest real component among the eigenvalues of the Jacobian matrix $\lambda_{\max} = \max \Re(\lambda(J))$. Negative values of the stability metric indicate locally asymptotically stable equilibria, whereas positive values correspond to unstable equilibria. A transition of the metric through zero is interpreted as the occurrence of a Hopf bifurcation.

To eliminate the computational cost associated with repeated eigenvalue evaluations during optimization, a feedforward neural network was developed to approximate the spectral abscissa as a smooth function of the system states and the bifurcation parameter. Hyperbolic tangent (Tanh) activation functions were employed because they provide continuous differentiability, making the surrogate model compatible with gradient-based optimization algorithms. The trained network therefore serves as a smooth and differentiable approximation of the stability metric, enabling its direct incorporation into optimal control formulations without requiring explicit eigenvalue calculations.

4. Results and Discussion

The bifurcation performed with MATCONT revealed the existence of a Hopf bifurcation point at (a_1, a_2, a_3, a_4, Da) values (0.678063 0.761589 1.947385 -1.917246 3.914244) with a first Lyapunov coefficient = 6.865616e-01. Figure. 1 shows the limit cycle.

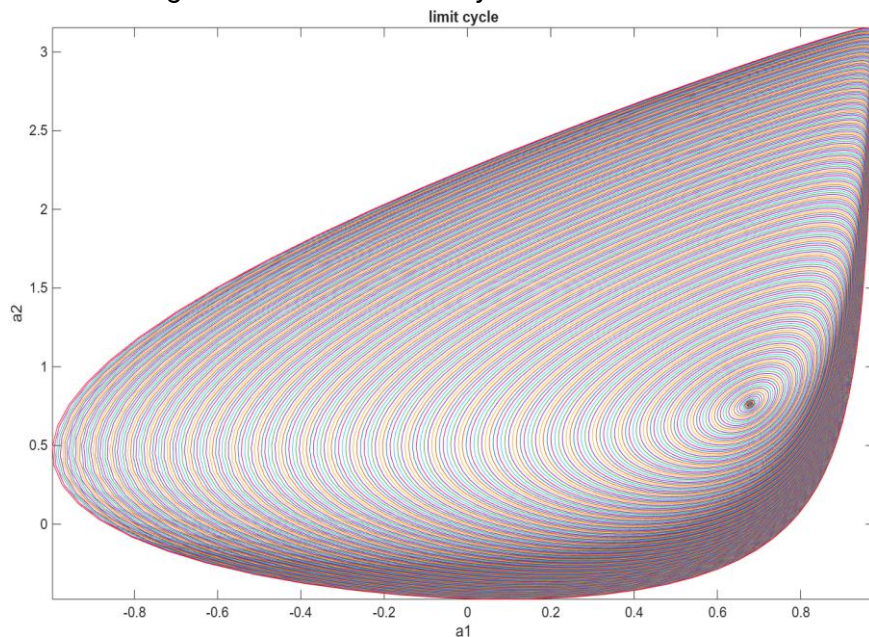


Figure 1. Limit Cycle

The analytical Jacobian is:

$$Ja = \begin{bmatrix} \sigma_1 + c_1 a_2 & -\omega + c_1 a_1 & \beta_1 & 0 \\ \omega + c_2 a_2 & \sigma_2 + c_2 a_1 & 0 & \beta_2 \\ c_3 b_1 & 0 & \gamma_1 + c_3 a_1 + Da - 3b_1^2 & 0 \\ 0 & c_4 b_2 & 0 & \gamma_2 + c_4 a_2 + Da - 3b_2^2 \end{bmatrix} \quad (11)$$

At the Hopf point, $(a_1, a_2, b_1, b_2, Da) = (0.678063, 0.761589, 1.947385, -1.917246, 3.914244)$ with parameters $\sigma_1 = -1, \sigma_2 = -1.2, \gamma_1 = 0.8, \gamma_2 = -1, \beta_1 = 0.6, \beta_2 = 0.5, \tau_1 = 2, c_2 = c_3 = c_4 = 1, \omega = 2$ the numerical Jacobian becomes.

$$J_n = \begin{bmatrix} 0.523178 & -0.643874 & 0.600000 & 0 \\ 2.761589 & -0.521937 & 0 & 0.500000 \\ 1.947385 & 0 & -7.584618 & 0 \\ 0 & -1.917246 & 0 & -7.351664 \end{bmatrix} \quad (12)$$

The eigenvalues of this matrix are $1.156i, 1.156i; -7.72$, and -7.21 . The presence of 2 complex conjugates on the imaginary axis confirms the existence of the Hopf bifurcation point. The soft penalty formulation involves minimizing oscillatory energy and control effort, and the original objective function is $\sum optv(t) = \sum (a_1(t))^2 + (a_2(t))^2 + (Da(t))^2$ with and without the Hopf bifurcation constraint. In a Hopf-type system, this typically suppresses oscillation amplitude and biases the dynamics toward the least-excited (often near-steady or weakly oscillatory) regime. To investigate the effect of bifurcation-aware operation, an optimal control problem was solved both with and without a Hopf-bifurcation-avoidance constraint using PYOMO.DAE coupled with IPOPT. PYOMO.DAE with IPOPT was used. When no Hopf constraint was implemented, $\alpha_{Hopf} = 0$, in $\sum (optv(t) + \alpha_{hopf} \cdot s_{max} (\lambda + \varepsilon_1))^2$ The obtained value of $\sum optv(t)$ was 183.306. For a Hopf constraint, $\alpha_{Hopf} = 3$, the obtained value of $\sum optv(t)$ was 17.975. This shows a considerable decrease in the minimized function, indicating the effect of the Hopf bifurcation constraint on minimizing anisotropy. This corresponds to approximately 90 % reduction in the minimized function value, demonstrating that enforcing Hopf-aware control strongly suppresses oscillatory energy. Figures 2 and 3 show the optimal control profiles without and with the Hopf constraint.

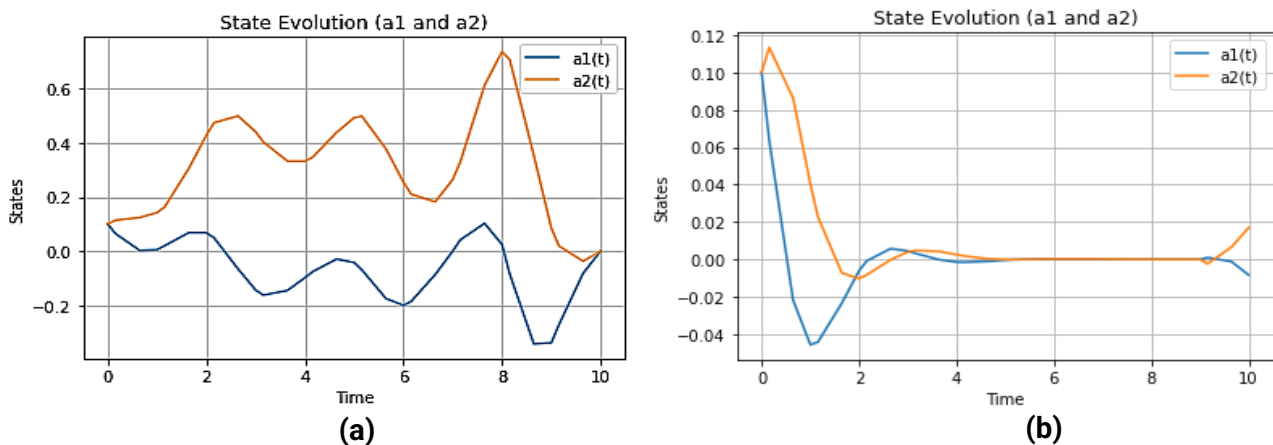


Figure 2. a_1 a_2 profiles without Hopf constraint

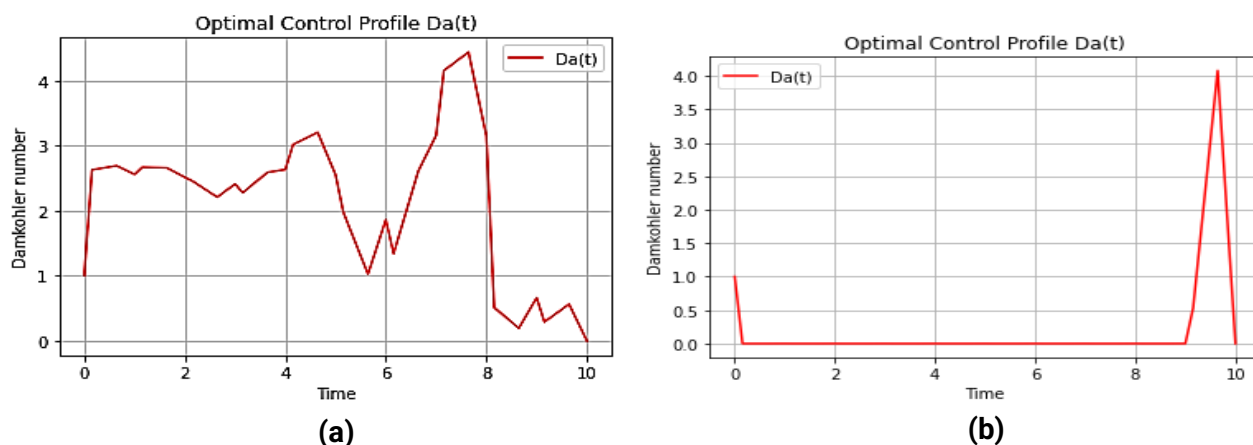


Figure 3. $Da(t)$ profile without the Hopf constraint

The reduced-order reacting fluid model exhibits rich nonlinear dynamics arising from the interaction between modal fluid motion, scalar transport, and nonlinear reaction kinetics. The system was analyzed using numerical continuation in MATCONT, which revealed the existence of a Hopf bifurcation at the parameter set:

$$(a_1, a_2, b_1, b_2, Da) = (0.678063, 0.761589, 1.947385, -1.917246, 3.914244),$$

with an associated first Lyapunov coefficient $l_1 = 6.865616 \times 10^{-1}$. The positive sign of the Lyapunov coefficient indicates that the Hopf bifurcation is subcritical in nature, implying the emergence of unstable limit cycles in the vicinity of the bifurcation point. This is consistent with the observation that the system transitions from a stable equilibrium branch to oscillatory dynamics via a finite-amplitude instability. The bifurcation structure suggests that nonlinear effects play a dominant role in shaping the post-critical behavior, and that oscillations may persist even in parameter regimes where the equilibrium is linearly stable [35].

The existence of a Hopf bifurcation is further confirmed by the eigenvalue structure of the linearized Jacobian at the critical point, where a complex conjugate pair crosses the imaginary axis while the remaining eigenvalues remain in the left half-plane. This separation of time scales indicates that the oscillatory instability is governed primarily by a two-mode interaction embedded within the four-dimensional reduced system. The resulting limit cycle, shown in Figure 2a, confirms the presence of sustained periodic oscillations in the reduced-order dynamics.

From a physical perspective, the oscillatory behavior can be interpreted as arising from the competition between reaction-driven growth, advective transport, and nonlinear saturation. The Damköhler number plays a central role in this balance, acting as the principal bifurcation parameter controlling the transition between steady and oscillatory regimes. At intermediate values of Da , reaction terms are sufficiently strong to destabilize the equilibrium, while nonlinear damping mechanisms are not yet dominant enough to suppress oscillations. This regime corresponds to the onset of Hopf instability and the emergence of self-sustained oscillatory energy exchange between velocity and scalar modes [36].

To investigate the possibility of controlling or suppressing these oscillations, an optimal control framework was introduced using Pyomo.DAE coupled with IPOPT. The control objective was formulated as a soft penalty problem that minimizes a combination of oscillatory energy and control effort. Specifically, the objective penalizes the integrated modal energy, thereby encouraging the system to evolve toward low-amplitude or weakly oscillatory states. In addition, a Hopf-bifurcation-avoidance

constraint was introduced to restrict the system dynamics away from parameter regimes associated with oscillatory instability.

The optimal control problem was solved in two configurations: (i) without the Hopf constraint and (ii) with the Hopf-aware constraint enforced. In the absence of the constraint, the system converged to a solution with an objective function value of 183.306. This corresponds to an unconstrained minimization of oscillatory energy, where the optimizer primarily balances intrinsic system dissipation against the imposed cost functional [37]. However, the resulting trajectory still exhibits significant residual oscillatory behavior, indicating that the optimization alone is insufficient to fully suppress the underlying instability mechanism.

In contrast, when the Hopf-bifurcation-avoidance constraint is imposed, the optimal solution undergoes a dramatic reduction in the objective function value to 17.975. This represents approximately a 90% reduction in the minimized cost, indicating a strong suppression of oscillatory energy and a significant shift in the system's dynamical regime. The constrained solution effectively steers the system away from the Hopf-active region of the parameter space, thereby preventing the amplification of oscillatory modes [38].

This result highlights an important interplay between bifurcation structure and optimal control. In particular, it demonstrates that incorporating knowledge of bifurcation boundaries into the control formulation can substantially enhance performance compared to unconstrained optimization. Rather than merely reacting to oscillations after they emerge, the Hopf-aware formulation actively reshapes the admissible state space, preventing the system from entering regimes where oscillatory instabilities are dynamically favored [10], [21].

From a dynamical systems perspective, the observed reduction in oscillatory energy can be interpreted as a suppression of the unstable manifold associated with the Hopf bifurcation. The control action effectively alters the effective Jacobian structure along the trajectory, reducing the tendency for complex eigenvalue pairs to approach the imaginary axis. This leads to a more strongly dissipative regime in which perturbations decay more rapidly and nonlinear mode interactions are weakened.

Overall, the results demonstrate that the reduced-order reacting fluid system not only captures classical Hopf bifurcation behavior but also provides a useful testbed for bifurcation-aware optimal control strategies. The substantial reduction in the objective function under the Hopf constraint suggests that explicitly incorporating stability boundaries into the control formulation can yield significant performance improvements, particularly in systems where oscillatory instabilities dominate the dynamics [7], [39].

he proposed framework for analyzing and controlling oscillatory instabilities in reacting fluid systems has broad implications for nonlinear dynamics, chemical engineering, and flow control. By combining reduced-order modeling, bifurcation analysis, and optimal control within a unified computational structure, the study provides a systematic approach for understanding and manipulating complex spatiotemporal behavior in reacting flows. The ability to capture Hopf bifurcations in a low-dimensional model offers a tractable yet physically meaningful representation of instability mechanisms that are otherwise accessible only through high-fidelity simulations.

From a theoretical perspective, the work contributes to the development of physics-informed reduced-order models that preserve essential nonlinear mechanisms responsible for oscillatory behavior. The identification of Hopf bifurcation structure within a chemically reacting flow context strengthens the connection between dynamical systems theory and transport-reaction phenomena. In particular, the explicit representation of modal interactions and reaction-induced feedback provides a clear interpretation of how energy transfer between flow and scalar fields leads to instability. This

enhances the understanding of subcritical and nonlinear bifurcation behavior in coupled fluid-chemical systems.

From a computational and methodological standpoint, the integration of MATCONT-based continuation analysis with PyomoDAE optimal control provides a powerful hybrid framework for studying nonlinear systems. The ability to compute bifurcation points, quantify stability through Lyapunov coefficients, and subsequently design control strategies that explicitly account for these structures represents a significant advancement in model-based control of nonlinear distributed systems. The introduction of bifurcation-aware constraints further demonstrates how stability information can be embedded directly into optimization problems, leading to improved performance and robustness compared to classical energy-based control formulations.

From an application perspective, the results are relevant to a wide range of chemical and fluid engineering systems where oscillatory instabilities are undesirable or must be controlled. Examples include reactive combustion systems, catalytic reactors, mixing-driven chemical processes, and environmental fluid systems such as eutrophication dynamics in water bodies. In such systems, oscillations can lead to reduced efficiency, unsafe operating conditions, or undesirable product distributions. The proposed methodology offers a pathway for suppressing or reshaping these oscillations through parameter-aware optimal control strategies.

In addition, the framework provides a foundation for future extensions toward data-driven and machine-learning-enhanced control of nonlinear fluid-reaction systems. By embedding the bifurcation structure into reduced-order models, it becomes possible to develop predictive control strategies that remain effective across parameter regimes that exhibit qualitative changes in dynamics. This is particularly important for real-world systems where operating conditions vary and stability margins are limited.

Overall, the proposed research advances both the theoretical understanding and practical control of nonlinear oscillatory phenomena in reacting flows, offering a scalable framework that bridges dynamical systems theory, chemical engineering applications, and modern optimal control techniques.

5. Conclusion

A nonlinear reduced-order model for a reacting fluid system was developed to investigate the onset of oscillatory instabilities and their suppression through optimal control. The model captures the essential coupling between velocity modes and scalar reaction dynamics through a four-dimensional system derived from modal truncation and physically motivated interaction terms. The inclusion of nonlinear convection, scalar-flow feedback, and cubic reaction kinetics enables the system to reproduce key features of reacting flow instabilities, including self-sustained oscillations and bifurcation-driven transitions. Numerical continuation using MATCONT revealed the existence of a Hopf bifurcation at:

$$(a_1, a_2, b_1, b_2, Da) = (0.678063, 0.761589, 1.947385, -1.917246, 3.914244)$$

with a positive first Lyapunov coefficient, indicating a subcritical Hopf bifurcation. The associated eigenvalue structure confirms the presence of a complex conjugate pair crossing the imaginary axis, leading to the emergence of a limit cycle, as verified numerically. This behavior highlights the intrinsic nonlinear mechanism by which reaction-transport imbalance induces oscillatory energy exchange between dominant flow and scalar modes.

An optimal control framework was then formulated using Pyomo.DAE with IPOPT, where the objective function minimizes oscillatory modal energy subject to system dynamics. A bifurcation-aware constraint was introduced to avoid operating regimes near the Hopf instability boundary. The results

demonstrate a significant improvement in system performance when the Hopf constraint is enforced. In particular, the objective function value decreased from 183.306 in the unconstrained case to 17.975 in the constrained case, corresponding to an approximate 90% reduction in oscillatory energy.

These results highlight the importance of incorporating nonlinear dynamical systems insights into optimal control formulations. Rather than treating oscillations as purely time-domain phenomena, the present approach leverages bifurcation structure to guide system behavior away from instability regions. The strong reduction in oscillatory energy demonstrates that Hopf-aware control can significantly enhance performance and robustness in nonlinear reacting flow systems.

Overall, the study establishes a computational framework combining reduced-order modeling, bifurcation analysis, and optimal control. This framework provides a foundation for future extensions to higher-dimensional fluid-reaction systems and offers a promising direction for stability-aware control of nonlinear distributed dynamical systems.

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APPENDIX

Table 1. Model variables (symbols, names, and units)

Symbol	Name / Physical meaning	Units
a_1	First velocity mode amplitude	$\text{m}\cdot\text{s}^{-1}$
a_2	Second velocity mode amplitude	$\text{m}\cdot\text{s}^{-1}$
b_1	First scalar (temperature/concentration) mode	$\text{kg}\cdot\text{m}^{-3}$ (or dimensionless)
b_2	Second scalar mode	$\text{kg}\cdot\text{m}^{-3}$ (or dimensionless)
c_1	Nonlinear velocity-velocity coupling coefficient	s^{-1}
c_2	Nonlinear velocity-velocity coupling coefficient	s^{-1}
c_3	Velocity-scalar coupling coefficient	s^{-1}
c_4	Velocity-scalar coupling coefficient	s^{-1}
β_1	Scalar forcing on velocity mode 1	s^{-1}
β_2	Scalar forcing on velocity mode 2	s^{-1}
σ_1	Linear damping (mode 1 velocity)	s^{-1}
σ_2	Linear damping (mode 2 velocity)	s^{-1}
γ_1	Linear damping (scalar mode 1)	s^{-1}
γ_2	Linear damping (scalar mode 2)	s^{-1}
Da	Damköhler number (reaction–transport ratio)	dimensionless
ω	Rotational coupling frequency	s^{-1}
t	Time	s

Table 2. Parameters (symbols, values, and units)

Symbol	Description	Value	Units
σ_1	Velocity mode 1 damping	-1.0	s^{-1}
σ_2	Velocity mode 2 damping	-1.2	s^{-1}
γ_1	Scalar mode 1 damping	-0.8	s^{-1}
γ_2	Scalar mode 2 damping	-1.0	s^{-1}
β_1	Coupling coefficient	0.6	s^{-1}
β_2	Coupling coefficient	0.5	s^{-1}
c_1	Nonlinear coupling	2.0	s^{-1}
c_2	Nonlinear coupling	1.0	s^{-1}
c_3	Scalar coupling	1.0	s^{-1}
c_4	Scalar coupling	1.0	s^{-1}
ω	Rotational frequency	2.0	s^{-1}
Da	Damköhler number at Hopf	3.914244	–
a_1^*	Hopf equilibrium value	0.678063	$\text{m}\cdot\text{s}^{-1}$
a_2^*	Hopf equilibrium value	0.761589	$\text{m}\cdot\text{s}^{-1}$
b_1^*	Hopf equilibrium value	1.947385	$\text{kg}\cdot\text{m}^{-3}$
b_2^*	Hopf equilibrium value	-1.917246	$\text{kg}\cdot\text{m}^{-3}$