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Article

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Bifurcation-Guided Optimal Control of Fluid Catalytic Cracking Systems with Productivity Enhancement

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ABSTRACT

Fluid catalytic cracking (FCC) is one of the most important processes in the petroleum and petrochemical industries because it converts heavy hydrocarbons into valuable transportation fuels and petrochemical feedstocks. However, FCC units exhibit highly nonlinear behavior, including multiplicity, thermal instability, Hopf bifurcations, and self-sustained oscillations, all of which can adversely affect catalyst performance, product yield, and operational stability. A nonlinear dynamic and optimal control framework is developed for an FCC process exhibiting bifurcation-induced instability. Continuation and bifurcation analyses are performed using MATCONT to identify limit points, Hopf bifurcation points, and associated limit-cycle behavior. Based on these analyses, an optimal control problem is formulated to maximize the cracking reaction rate while incorporating a Hopf-bifurcation-avoidance constraint to ensure dynamically stable operation. The bifurcation analysis reveals multiple steady states and a subcritical Hopf bifurcation, confirming the onset of self-sustained oscillatory dynamics in the FCC process. The optimal control results demonstrate that enforcing the Hopf bifurcation constraint significantly improves process performance. Specifically, the optimized cracking reaction rate increases from 6.254 in the unconstrained case to 7.443 when the Hopf constraint is imposed, corresponding to an approximately 19% improvement while maintaining dynamic stability. The proposed framework demonstrates that integrating bifurcation analysis with optimal control provides an effective strategy for simultaneously enhancing process stability and operational performance in FCC systems. The results highlight the industrial significance of incorporating nonlinear dynamic constraints into process optimization to achieve safer, more efficient, and higher-performing FCC operation.

1. Introduction

Fluid catalytic cracking (FCC) remains one of the most important conversion processes in petroleum refining, where heavy hydrocarbon fractions are transformed into valuable products such as gasoline, light olefins, and other transportation fuels. Due to the strong coupling between reaction kinetics, catalyst circulation, heat transfer, and regeneration phenomena, FCC units exhibit highly nonlinear dynamic behavior that requires accurate mathematical modeling and advanced control strategies. Early dynamic simulation studies established the importance of rigorous reactor-regenerator models for predicting transient behavior and evaluating operational strategies in industrial FCC units [1].

The development of comprehensive FCC dynamic models enabled the analysis of process interactions, operating constraints, and control limitations in commercial FCC systems. McFarlane et al. developed a dynamic simulator for a Model IV FCC unit, demonstrating the importance of integrated reactor and regenerator dynamics for realistic process prediction [1]. Arbel et al. presented a systematic three-part investigation of FCC dynamics, including detailed mathematical modeling, nonlinear steady-state behavior, instability mechanisms, and design considerations for improved controllability [2], [3], [4]. These studies demonstrated that FCC units can exhibit multiple steady states

and complex nonlinear responses due to the coupling between catalyst activity, reaction rates, and thermal effects [3], [4].

Dynamic optimization and integrated process modeling approaches have further improved the understanding of FCC operation. Gani and Cameron introduced integrated dynamic modeling and optimization methodologies for FCC units, highlighting the importance of simultaneous consideration of process dynamics and operating objectives [5]. Bifurcation-based investigations revealed that FCC reactors may undergo transitions between stable and unstable operating regimes, with static and dynamic bifurcations playing an important role in determining safe operating windows [6]. Such nonlinear phenomena motivate the development of stability-aware optimization frameworks capable of identifying and avoiding undesirable operating conditions.

Nonlinear modeling and advanced control have been extensively investigated to address the challenges associated with FCC operation. Romagnoli and Palazoglu developed nonlinear FCC reactor models and demonstrated the limitations of conventional linear control approaches for highly nonlinear refining systems [7]. Han and Chung proposed nonlinear predictive control strategies for FCC processes, showing improved performance under changing operating conditions and process constraints [8]. Mathematical modeling, simulation, and optimization studies by Elnashaie and Elshishini further emphasized the importance of nonlinear reactor representations for understanding FCC behavior and improving process operation [9].

Steady-state multiplicity represents one of the fundamental nonlinear characteristics of FCC reactors. Chang and Whiting analyzed multiplicity phenomena in FCC systems and demonstrated the influence of operating parameters on the existence of multiple equilibrium solutions [10]. These results established the need for stability analysis tools that can distinguish desirable operating points from unstable regions.

Advanced control strategies have continued to evolve with the objective of improving FCC efficiency, reliability, and product quality. Moro and Odloak investigated constrained multivariable control of FCC units, demonstrating the challenges associated with manipulating multiple interacting process variables while satisfying operational constraints [11]. Fernandes and Oliveira developed nonlinear control structure design methodologies specifically for FCC processes, emphasizing the need for control approaches capable of handling strong nonlinearities [12]. Industrial-scale modeling efforts by McGreavy and Santos provided additional insight into fluidized catalytic cracking reactor behavior and highlighted the importance of accurate hydrodynamic and kinetic descriptions [13].

Riser reactor modeling and kinetic analysis have also been central components of FCC research. de Lasa and Kumar investigated riser modeling approaches and reaction kinetics, providing improved understanding of catalyst-hydrocarbon interactions and their influence on reactor performance [14]. Dynamic optimization studies by Ali and Rohani demonstrated that optimal operating strategies can significantly improve FCC performance while accounting for dynamic process behavior [15]. Model predictive control approaches were subsequently applied to FCC systems to address constraints and enhance regulatory performance under industrial operating conditions [16].

The stability characteristics of FCC reactors have received increasing attention because unstable operation can lead to reduced conversion efficiency and operational risks. Elkamel and Budman investigated bifurcation and stability behavior in FCC reactors, showing the importance of nonlinear stability analysis for identifying critical operating conditions [17]. Tang and Forbes developed nonlinear control and real-time optimization strategies, demonstrating the potential of advanced optimization methods for improving FCC operation [18].

Comprehensive reviews have summarized decades of progress in FCC modeling, simulation, and control. Pinheiro et al. reviewed FCC process modeling, simulation, and control approaches, emphasizing the transition from conventional empirical models toward more rigorous nonlinear and computational frameworks [19]. Fernandes and Pinheiro further explored nonlinear dynamics and optimization of FCC systems, highlighting the importance of combining dynamic modeling with optimization techniques for improved operation [20].

Recent research has expanded FCC modeling toward catalyst science, digital technologies, and artificial intelligence-based approaches. Vogt and Weckhuysen reviewed recent developments in FCC catalyst technology and emphasized the continuing importance of FCC in modern refining operations [21]. The integration of artificial intelligence and data-driven methods has opened new possibilities for FCC prediction, optimization, and control by enabling nonlinear relationships to be captured from process data [22]. Machine learning and computational intelligence approaches are increasingly being investigated as complementary tools to traditional mechanistic modeling approaches for complex chemical processes [22].

The development of advanced FCC optimization strategies requires integration with broader process systems engineering methodologies. Process dynamics and control frameworks provide the theoretical foundation for designing robust nonlinear controllers and optimization algorithms for complex chemical systems [23], [24]. Process design methodologies further support the integration of reaction engineering, transport phenomena, and optimization principles for developing efficient industrial processes [25].

A growing body of recent research has focused on integrating artificial intelligence, digital twins, and physics-informed machine learning into chemical process systems to enable more reliable, efficient, and intelligent process operation. Hao et al. [26] presented a comprehensive review of physics-informed machine learning methodologies, highlighting how the incorporation of governing physical laws into data-driven models significantly improves prediction accuracy, model robustness, and generalization while reducing dependence on large experimental datasets. These developments demonstrate the potential of physics-informed approaches for complex nonlinear chemical engineering systems. Building upon this concept, Arce Muñoz and Hedengren [27] developed a physics-informed transfer learning framework for process control applications, showing that combining first-principles knowledge with machine learning enhances controller performance, accelerates model adaptation, and improves optimization in dynamic industrial processes. The emergence of digital twin technology has further expanded opportunities for real-time process optimization. Pal *et al*. reviewed recent advances in digital twins for the chemical process industry and demonstrated their growing importance in online monitoring, predictive maintenance, process optimization, soft sensing, and operational decision support [28]. Their review emphasized that digital twins provide a powerful platform for integrating mechanistic models, process measurements, and artificial intelligence to improve plant efficiency and reliability. Similarly, Weingram and Cui proposed a comprehensive taxonomy of digital twins and illustrated how the integration of machine learning with high-fidelity physical models enables continuous system updating, improved predictive capability, and intelligent decision-making across engineering applications [29].

Collectively, these recent studies indicate that future chemical process optimization will increasingly rely on hybrid frameworks that combine first-principles modeling, artificial intelligence, and real-time digital representations of industrial systems. The present work complements these developments by incorporating nonlinear bifurcation analysis and stability-aware optimal control into an FCC process, thereby providing a physics-based framework capable of achieving improved productivity while maintaining dynamically stable operation.

Despite significant progress, existing FCC studies have primarily focused on modeling, control, and optimization separately. A unified framework that combines nonlinear dynamic analysis, bifurcation detection, and optimal operation remains an important research opportunity. In particular, stability-aware optimization approaches based on Hopf bifurcation analysis can provide a systematic methodology for identifying safe operating regions and preventing oscillatory instabilities in FCC systems.

A major objective of the study is to identify and characterize the nonlinear bifurcation structure of the FCC model. In particular, the work focuses on detecting limit points and Hopf bifurcation points using continuation techniques implemented in MATCONT. Identifying these bifurcation points is important because they determine the boundaries between stable and unstable operating regimes. Special attention is devoted to the analysis of Hopf bifurcation behavior, since the onset of oscillatory dynamics can lead to undesirable limit-cycle operation in industrial FCC units. The study, therefore, seeks to understand how variations in the air-flow operating parameter influence the transition from steady-state behavior to self-sustained oscillations.

The novelty of this work lies in integrating nonlinear bifurcation analysis with dynamic optimal control for a fluid catalytic cracking (FCC) process within a unified computational framework. Unlike conventional FCC optimization studies that focus solely on maximizing process performance, the proposed methodology explicitly incorporates Hopf bifurcation avoidance to ensure that the computed optimal operating conditions remain dynamically stable. By combining MATCONT-based continuation analysis, limit cycle computation, and bifurcation-constrained optimal control, the proposed approach establishes a direct relationship between nonlinear stability and industrial productivity. The results demonstrate that avoiding oscillatory operating regimes leads to an approximately 19% increase in the cracking reaction rate, highlighting the significant industrial benefits of stability-aware optimization. To the best of the author's knowledge, this is among the first studies to directly couple Hopf bifurcation theory with optimal control for FCC systems, providing a practical framework for improving both productivity and operational reliability in large-scale industrial chemical processes.

2. Research and Methodology

Consider a lumped nonlinear dynamic model of a fluid catalytic cracking (FCC) unit consisting of a riser reactor and regenerator coupled through catalyst circulation. The principal state variables are the riser temperature T_r, regenerator temperature T_g, coke concentration on spent catalyst C_c, oxygen concentration in the regenerator O_2, and catalyst circulation rate F_c. The manipulated variables are the regenerator air flow rate F_{air} and feed preheat temperature T_f. The nonlinear interactions among cracking reactions, coke deposition, combustion, and catalyst recirculation generate oscillatory dynamics that can undergo a Hopf bifurcation.

The riser reactor energy balance is written as

$$\frac{dT_r}{dt} = \frac{F_f C_{pf}\left(T_f - T_r\right) + F_c C_{pc}\left(T_g - T_r\right) + \left(-\Delta H_r\right) R_r V_r}{M_r C_{pr}} \tag{1}$$

Where F_f is the feed flow rate, C_{pf} is the feed heat capacity, C_{pc} is the catalyst heat capacity, $M_r$is the effective riser mass, $C_{pc}$is the riser heat capacity, ΔH_r is the heat of cracking reaction, R_r is the cracking reaction rate, and V_r is the riser volume. The cracking kinetics are modeled using Arrhenius behavior,

$$R_r = k_r \exp(-\frac{E_r}{RT_r}) C_f \tag{2}$$

where k_r is the pre-exponential factor, E_r is the activation energy, R is the universal gas constant, and C_f is the feed hydrocarbon concentration. The coke deposition dynamics on the catalyst are described by:

$$\frac{dC_c}{dt} = Y_c R_r - \frac{F_c}{M_c} C_c - R_b \tag{3}$$

where Y_c is the coke yield coefficient, M_c is the catalyst inventory, and R_b is the coke combustion rate in the regenerator. The regenerator energy balance is:

$$\frac{dT_g}{dt} = \frac{F_c C_{pc}\left(T_r - T_g\right) + \left(-\Delta H_b\right) R_b V_g + F_{air} C_{pa}\left(T_{air} - T_g\right)}{M_g C_{pg}} \tag{4}$$

where V_g is the regenerator volume, M_g is the regenerator mass inventory, C_{pg} is the regenerator heat capacity, C_{pa} is the air heat capacity, T_{air} is the inlet air temperature, and ΔH_b is the heat released during coke combustion. The coke combustion kinetics are modeled as:

$$R_b = k_b \exp(|\frac{E_b}{RT_g}) C_c O_2 \tag{5}$$

where k_b is the combustion pre-exponential factor and E_b is the combustion activation energy. The oxygen balance in the regenerator is given by:

$$\frac{dO_2}{dt} = \frac{F_{air}}{V_g}\left(O_{2,in} - O_2\right) - \nu_b R_b \tag{6}$$

where $O_{2,in}$ is the inlet oxygen concentration and ν_b is the stoichiometric oxygen consumption coefficient. The catalyst circulation dynamics are represented by a first-order nonlinear actuator model,

$$\frac{dF_c}{dt} = \frac{1}{\tau_c}\left(F_{c,set} - F_c\right) - \alpha_c\left(T_g - T_r\right) \tag{7}$$

where $F_{c,set}$ is the desired catalyst circulation rate, τ_c is the circulation response time constant, and α_c is the thermal coupling coefficient accounting for temperature-driven circulation effects. The nonlinear FCC dynamic model may therefore be compactly expressed as:

$$\frac{dx}{dt} = f\left(x, u, p\right) \tag{8}$$

where the state vector is $x = [T_r, T_g, C_c, O_2, F_c]^T$ and the control vector is $u = [F_{air}, F_{c,set}, T_f]^T$ and the parameter vector p contains the kinetic, thermodynamic, transport, and geometric parameters of the FCC unit.

The model needs to be scaled because the original FCC nonlinear system contains variables that differ by several orders of magnitude (temperatures in 10^2 - 10^3 K, reaction rates in large exponential ranges, and concentrations in $O(1)$, which leads to ill-conditioning in Newton-based solvers, poor Jacobian scaling, and unreliable bifurcation detection near Hopf points. Scaling also ensures that all state variables evolve on comparable numerical ranges, which is essential for robust convergence of fsolve, accurate eigenvalue tracking, and stable training of reduced-order neural models. In addition,

scaling improves interpretability of the bifurcation parameter by normalizing operational deviations around a physically meaningful steady operating point.

To achieve this, a nondimensional transformation is introduced for the principal state variables. Temperatures are shifted and scaled around nominal FCC operating conditions, while concentrations and flow variables are normalized by characteristic magnitudes. The scaled states are defined as $\theta_r = (T_r - 700)/100$, $\theta_g = (T_g - 750)/100$, $c = C_c$, $o = O_2$, and $f = F_c/5$, while the manipulated and bifurcation input is normalized as $u = F_{air}/10$. The inverse transformations are $T_r = 700 + 100\theta_r$, $T_g = 750 + 100\theta_g$, $F_c = 5f$, and $F_{air} = 10u$. This choice ensures that all state variables remain $O(1)$ in magnitude, which significantly improves numerical conditioning and preserves nonlinear structure required for Hopf bifurcation.

Using these scaled variables, the FCC system can be written in continuous form as follows:

$$\frac{d\theta_r}{dt} = \frac{1}{100 M_r C_{pc}} (F_f C_{pf} (T_f - (700 + 100\theta_r)) + (5f) C_{pc} ((750 + 100\theta_g) - (700 + 100\theta_r)) + (-\Delta H_r) R_r V_r) \tag{9}$$

$$\frac{d\theta_g}{dt} = \frac{1}{100 M_g C_{pg}} [(5f) C_{pc} ((700 + 100\theta_r) - (750 + 100\theta_g)) + (-\Delta H_b) R_b V_g + (10u) C_{pa} (T_{air} - (750 + 100\theta_g))] \tag{10}$$

$$\frac{dc}{dt} = Y_c R_r - \frac{5f}{M_c} c - R_b \tag{11}$$

$$\frac{do}{dt} = \frac{10u}{V_g} (O_{2,in} - o) - \nu R_b \tag{12}$$

$$\frac{df}{dt} = \frac{1}{\tau_c} (1 - f) - \alpha_c ((750 + 100\theta_g) - (700 + 100\theta_r)) \tag{13}$$

The nonlinear reaction rates are expressed in Arrhenius form consistent with the scaled temperature variables:

$$R_r = k_r \exp\left(-\frac{E_r}{R(700 + 100\theta_r)}\right)(0.2 + c) \tag{14}$$

$$R_b = k_b \exp\left(-\frac{E_b}{R(750 + 100\theta_g)}\right) c \max(o, 0.05) \tag{15}$$

This formulation preserves the full nonlinear coupling structure of the FCC system while ensuring numerical robustness for steady-state computation, bifurcation analysis, Neural ODE surrogate modeling, and nonlinear MPC design near Hopf instability regimes.The modifications to R_r and c are necessary to prevent numerical extinction of the reaction dynamics at low temperatures or near steady-state initialization, where the original formulation can drive $R_r \to 0$ and collapse the nonlinear coupling structure. Introducing a shifted coke term $(0.2 + c)$ ensures a baseline reaction activity so the system remains dynamically connected and capable of exhibiting Hopf bifurcation behavior. Similarly, smoothing the Arrhenius-driven R_r avoids sharp loss of reactivity that would otherwise eliminate feedback between thermal and material balances.

The objective of the present work is to investigate the nonlinear dynamic behavior and stability-aware optimal control of a reduced-order fluid catalytic cracking (FCC) model rather than to develop a detailed plant simulator for quantitative process prediction. Accordingly, the governing equations and kinetic relationships were formulated based on well-established dynamic FCC models reported in the literature, particularly the pioneering studies [2], [6], [19]. The model successfully reproduces the characteristic nonlinear behavior reported for industrial FCC systems, including multiple steady states, limit points, Hopf bifurcations, and self-sustained oscillatory dynamics, which have been widely documented in previous theoretical and industrial investigations. Furthermore, the predicted bifurcation structure and dynamic responses are consistent with the qualitative behavior reported in these benchmark studies, providing confidence that the reduced-order model captures the essential nonlinear physics governing FCC operation. Since the primary contribution of this work is the integration of bifurcation analysis with optimal control, detailed validation against plant measurements was beyond its scope. Nevertheless, extending the proposed framework to industrial FCC data or high-fidelity CFD and digital twin models represents an important direction for future research and would further demonstrate the practical applicability of the methodology.

2.1. Bifurcation Analysis and Optimal Control

2.1.1. 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], [31], [32]. This program identifies Limit points(LP), branch points(BP), and Hopf bifurcation points(H) for a dynamic system of ordinary differential equations.

2.1.2. Optimal Control

Pyomo.DAE is used for the Optimal Control calculations [33]. 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].

2.2 Formation of stability Dataset from MATCONT results

A stability dataset was developed from numerical continuation calculations performed in MATCONT. The stability dataset consists of rows, each representing a continuation point from an equilibrium branch. Each row contains the state variables, the bifurcation parameter, and a stability measure. The stability measure is a numerical value derived from the Jacobian matrix. The Jacobian matrix is computed numerically at each equilibrium point. The eigenvalues are then computed automatically using MATLAB. The maximum value of the real part of these eigenvalues is then computed as a scalar stability measure.

The stability measure is computed using “eig_real_max = max(real(eigvals));” in MATLAB. The stability measure is a quantitative metric in which negative values indicate locally asymptotically stable equilibria, positive values indicate instability, and a zero crossing indicates a Hopf bifurcation. The stability dataset is then saved as a CSV file. The dataset can then be used in subsequent computational

calculations to perform classification or regression to identify stability boundaries or approximate bifurcations.

2.3. Neural Network Surrogate for Stability Prediction

Before neural-network training, all input variables were standardized to improve numerical conditioning and training stability. Let x_{raw}denote the vector of state variables and bifurcation parameters= obtained from the stability dataset. For each input variable j, the training mean $\mu_j$and training standard deviation $\sigma_j$were computed over all training samples. = The training mean for the input variable j is defined as the arithmetic average over all training samples 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: $\sigma_j = \frac{1}{N}(\sum_{k=1}^{N} x_j^{(k)} - \mu_j)^2$. The standardized inputs are:

$$x_j = \frac{x_{raw,j} - \mu_j}{\max(\sigma_j, \varepsilon_{scale})} \tag{16}$$

where $\varepsilon_{\mathrm{scale}}$is a small positive regularization parameter introduced to prevent numerical singularities associated with extremely small variances. This transformation ensures that all inputs remain properly scaled while avoiding excessively large neural-network activation arguments during optimization. The normalization procedure improves neural-network conditioning and enhances the robustness of gradient-based optimization. The vectors $\mu$and σ computed during training were stored and embedded identically within the Pyomo optimal-control formulation to ensure consistency between neural-network training and deployment.

A feedforward neural network is trained to approximate the maximum eigenvalue as a smooth function of the system state and bifurcation parameter. A typical architecture employs the hyperbolic tangent $(\tanh)$ as a smooth activation function. If the input vector is denoted by x, which represents the scaled variables, then the network is defined as:

The vectors μ, σ computed during training were stored and embedded identically within the Pyomo optimal control formulation to ensure consistency between neural network training and deployment.

A feedforward neural network is trained to approximate the maximum real eigenvalue as a smooth function of the system states and bifurcation parameter, with hyperbolic tangent activation functions, ensuring smooth differentiability required by IPOPT. If the input vector is denoted by x, which are the scaled variables, the network architecture is defined as

$$\begin{aligned} z1 &= tanh\left(W1\,x + b1\right) \\ z2 &= tanh\left(W2\,z1 + b2\right) \\ \lambda\_max\_NN &= W3\,z2 + b3 \end{aligned} \tag{17}$$

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 z1, z2, represent nonlinear combinations of the inputs and previous-layer features, respectively. Each element of $z_1$is a smoothed combination of the original inputs, while each

element of z2 encodes more abstract patterns extracted from z1. The final output λ_max_NN provides a smooth approximation of the maximum real eigenvalue, enabling efficient and differentiable stability evaluation within the optimal control problem. The integration into optimal control is done using a soft penalty formulation where we use a smooth_max function that converts λ into a smooth, nonnegative penalty that only "activates" when the system is unstable:

$$s_{\max}(\lambda+\varepsilon_1) = smooth - \max(\lambda+\varepsilon_1) = \frac{(\lambda+\varepsilon_1)+\sqrt{(\lambda+\varepsilon_1)^2+\varepsilon_1}}{2} \quad (18)$$

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:

$optv(t) = \sum(Rr(t))$ is modified to $\sum(optv(t) + \alpha_{hopf}.s_{\max}(\lambda+\varepsilon_1))^2$ α_{Hopf}

controls how aggressively instability is penalized, and ε_1 prevents numerical issues at exactly λ = 0 and slightly shifts the stability boundary. The goal is to maximize the objective function value while ensuring differentiability for IPOPT and avoiding non-smooth optimization. Rr is the Cracking reaction rate. To facilitate integration into optimal control, a stability dataset is constructed from MATCONT continuation results. At each equilibrium point, the Jacobian is evaluated and its eigenvalues computed. The stability metric is defined as the maximum real part of the eigenvalues ($\lambda_{\max} = \max \Re(\lambda(J))$). Negative values indicate stability, positive values indicate instability, and zero crossings correspond to Hopf bifurcations.

3. Results and Discussion

Bifurcation analysis was performed using MATCONT with the air-flow parameter u selected as the continuation (bifurcation) parameter and setting $F_{air} = 10 * u$. A Hopf bifurcation point was detected with a first Lyapunov coefficient of 6.372120e-01, indicating a subcritical Hopf bifurcation. This bifurcation occurs at the equilibrium point at $[\theta_r;\theta_g,c,o,f,u]$ values of (35.667200; 32.942052; 0.004335; 0.239924; 106.456231; 3.538666). In addition, a limit point was located at $[\theta_r;\theta_g,c,o,f,u]$ values of (34.373884; 31.689964; 0.004263; 0.239929; 104.724671; 3.540739), indicating the presence of multiple steady states and a turning point in the equilibrium branch. The corresponding bifurcation diagram is shown in Figure 1. Continuation of the Hopf point reveals the existence of a limit cycle, confirming the emergence of self-sustained oscillatory dynamics in the system. The resulting periodic orbit is presented in Figure 2.

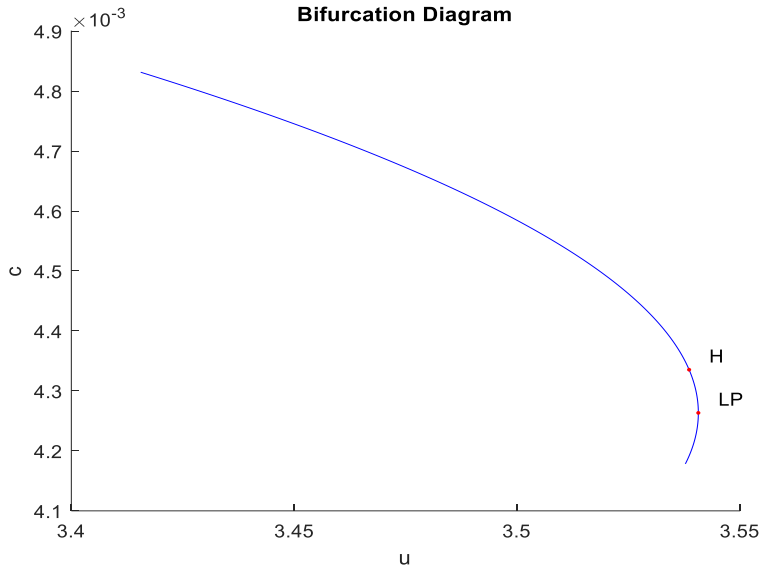

Figure 1. Bifurcation Diagram

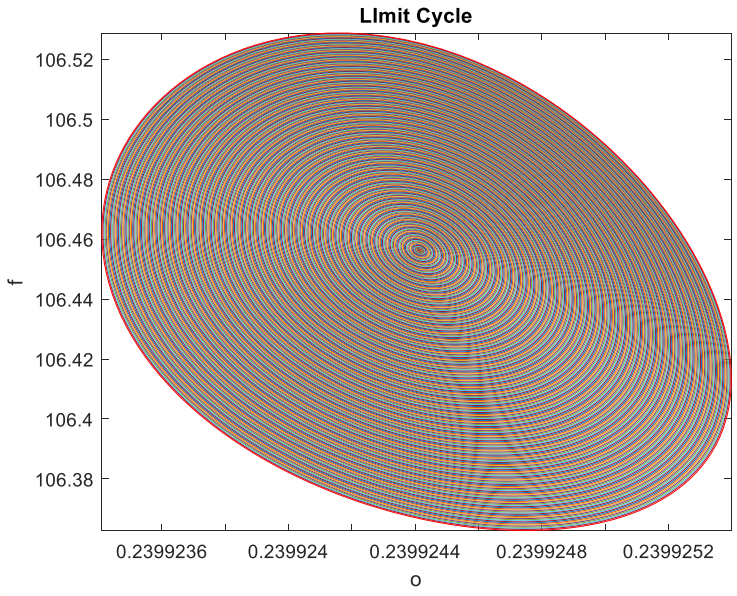

Figure 2. Limit cycle caused by Hopf Bifurcation

In the optimal control problem, the cracking reaction rate was maximized both without and with the Hopf bifurcation constraint. The objective function was defined as the maximization of the cracking reaction rate, $R_r = k_r e^{-\frac{E_r}{RT_r}}(0.6+c)$ over the specified time horizon. The objective function is $\sum((optv(t) = Rr(t)) + \alpha_{hopf}.s_{\max}(\lambda + \varepsilon_1))^2$. In the absence of the Hopf bifurcation constraint (α_{Hopf} = 0), the obtained optimal value of the $\sum((optv(t) = Rr(t))$ was 6.254. When the Hopf bifurcation avoidance constraint was activated with α_{Hopf} = 100 the value of $\sum((optv(t) = Rr(t))$ was increased to 7.443. This represents an approximate 19% improvement in the cracking reaction rate.

These results demonstrate that avoiding the Hopf bifurcation and the associated limit cycle oscillations can significantly enhance reactor productivity and operational performance in fluid catalytic

cracking systems. From an industrial perspective, suppressing oscillatory behavior improves process stability, reduces undesirable fluctuations, and allows operation in a more efficient regime. The comparison clearly shows the stabilizing effect of the Hopf-aware optimal control strategy and its positive impact on the achievable cracking performance. Figures 3-6 illustrate the optimal state and control trajectories obtained both without and with the Hopf bifurcation constraint.

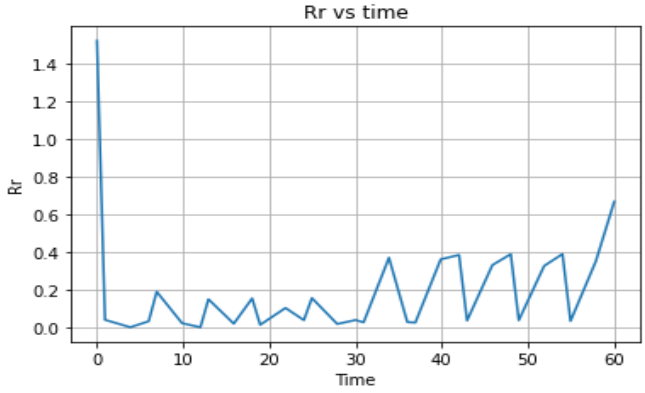

Figure. 3. Optimal control profile Rr vs time (no Hopf constraint)

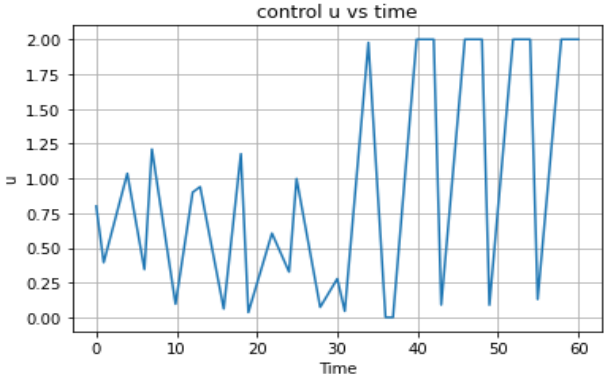

Figure. 4. Optimal control profile u vs time (no Hopf constraint)

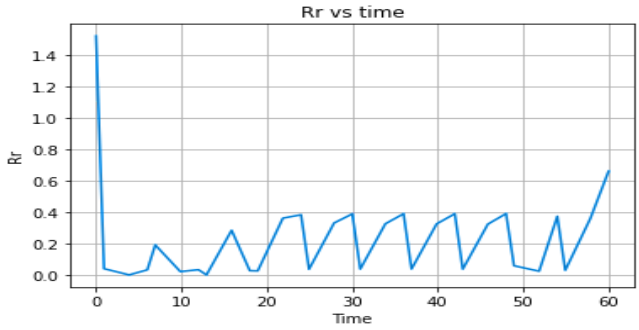

Figure. 5 Optimal control profile Rr vs time (with Hopf constraint)

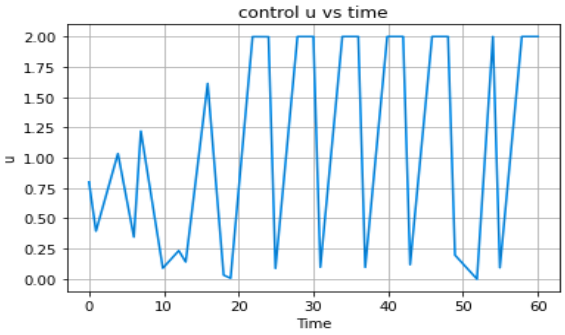

Figure. 6. Optimal control profile u vs time (with Hopf constraint)

The obtained results demonstrate the strong interaction between nonlinear dynamic behavior, process stability, and optimal operational performance in fluid catalytic cracking systems. The bifurcation analysis revealed the existence of both a limit point and a Hopf bifurcation, indicating that the FCC process possesses multiple steady states and oscillatory operating regimes over realistic operating conditions. Such behavior is highly significant from an industrial standpoint because FCC units are among the most economically important conversion processes in petroleum refineries, and unstable reactor-regenerator dynamics can substantially reduce process efficiency, catalyst performance, and operational safety.

The detection of a limit point indicates the presence of multiplicity in the steady-state solutions. In industrial FCC operation, multiplicity is particularly important because small changes in manipulated variables, feed conditions, or catalyst activity may force the system to transition abruptly between operating branches. Such transitions can produce severe thermal excursions, unstable regenerator operation, and undesirable variations in product quality. The existence of a turning point therefore highlights the narrow operating margins that may exist in highly nonlinear FCC processes. The present results demonstrate that the proposed model is capable of reproducing these important nonlinear

aoscillatory operation in the FCC system. The computed periodic orbit demonstrates that the observed oscillations are not merely transient numerical artifacts but correspond to stable nonlinear dynamic behavior supported by the governing process equations. This observation is important because many industrial process control strategies are designed based on local steady-state assumptions and may fail to adequately address nonlinear oscillatory phenomena. The present work therefore emphasizes the necessity of incorporating nonlinear dynamic analysis into advanced process operation and optimization frameworks.

A major contribution of this work is the integration of bifurcation analysis with optimal control. Rather than treating process stability and process optimization as separate tasks, the present framework directly links the suppression of instability with improved reactor performance. The obtained results clearly demonstrate that enforcing Hopf bifurcation avoidance during optimization produces a substantial increase in the cracking reaction rate. Specifically, the optimized cracking rate increased from 6.254 to 7.443 when the Hopf constraint was activated, corresponding to an improvement of approximately 19%. This improvement is industrially significant because even modest increases in FCC conversion efficiency can translate into substantial economic gains at refinery scale.

The improvement obtained under the Hopf-constrained optimization framework suggests that oscillatory operating regimes may inherently reduce effective cracking performance. Although oscillatory dynamics can temporarily increase local reaction intensities, sustained nonlinear oscillations often produce inefficient overall operation because the reactor-regenerator system repeatedly deviates from its optimal operating conditions. By constraining the optimization problem away from the Hopf bifurcation region, the proposed methodology drives the process toward dynamically stable operating regimes that simultaneously maintain high cracking activity and improved operational consistency.

From a control engineering perspective, the proposed methodology offers several practical advantages. First, the bifurcation-aware optimization framework provides a systematic approach for identifying operationally safe regions before implementing advanced controllers in industrial FCC units. Second, the approach can potentially reduce the likelihood of unexpected oscillatory transitions during plant disturbances or feedstock variations. Third, the framework may improve long-term catalyst utilization by reducing excessive coke accumulation and thermal cycling effects associated with unstable operation. These factors collectively contribute to improved plant reliability, enhanced energy efficiency, and reduced operational costs.

Another important aspect of this work is the computational strategy itself. The coupling of continuation methods with dynamic optimization provides a unified methodology for studying highly nonlinear chemical processes. Traditional optimization approaches may identify operating points that appear optimal locally but are dynamically unstable when implemented in practice. In contrast, the present approach explicitly incorporates nonlinear stability considerations into the optimization formulation. As a result, the computed optimal solutions are not only economically attractive but also dynamically meaningful and operationally feasible. This is particularly important for large-scale industrial processes where unstable operation can lead to significant economic penalties and operational risk.

The proposed framework also has broader implications beyond FCC systems. Many industrial chemical processes exhibit nonlinear dynamics, multiplicity, and oscillatory behavior, including polymerization reactors, combustion systems, biochemical reactors, electrochemical systems, and multiphase catalytic reactors. Consequently, the methodology developed in this work may be extended to a wide range of nonlinear process systems in which bifurcation-induced instability limits achievable

performance. The integration of bifurcation analysis with optimal control therefore represents a promising direction for the development of next-generation intelligent process operation strategies.

The present study does not employ a neural network or any data-driven surrogate model. Instead, the optimal control problem is solved directly using the governing nonlinear dynamic equations, while bifurcation analysis is performed using MATCONT. Consequently, the optimization results are obtained from the first-principles model without approximation by machine learning techniques. The objective of this work is to demonstrate the integration of nonlinear bifurcation analysis with optimal control for FCC systems. The incorporation of neural network surrogates, physics-informed machine learning, uncertainty quantification, and sensitivity analysis represents an important extension of the proposed methodology and is the subject of ongoing research. Although the present study demonstrates the effectiveness of the proposed stability-aware optimal control framework, a comprehensive sensitivity and uncertainty analysis was beyond the scope of the current work. The bifurcation behavior and optimal operating policy are expected to depend on parameters such as reaction kinetics, catalyst circulation rate, activation energies, and control weighting coefficients. Future work will investigate both local and global sensitivity analysis together with uncertainty quantification to assess the influence of parameter variability on the predicted Hopf bifurcation location, optimal control trajectories, and reactor productivity. Such analyses will further establish the robustness of the proposed methodology under realistic industrial operating conditions.

The obtained results demonstrate that incorporating nonlinear dynamic stability into the optimal control formulation can substantially improve FCC performance while maintaining stable reactor operation. The approximately 19% increase in the optimized cracking reaction rate achieved through Hopf bifurcation avoidance is significant when compared with previous FCC optimization studies, which have primarily focused on maximizing conversion, gasoline yield, or economic objectives without explicitly considering dynamic stability. Earlier investigations established the existence of multiple steady states and oscillatory behavior in FCC units [2], [4], while subsequent studies developed advanced control and optimization strategies to improve process performance [16], [18], [20]. However, these approaches generally did not incorporate bifurcation constraints to ensure operation away from oscillatory instability. More recently, Khaldi et al. emphasized the growing role of artificial intelligence and advanced optimization techniques for FCC systems but also highlighted the need for methodologies that simultaneously address productivity, process stability, and operational reliability [22]. The present work contributes to this emerging research direction by explicitly integrating Hopf bifurcation analysis with dynamic optimal control. From an industrial perspective, operating away from Hopf bifurcation points not only increases the cracking reaction rate but also suppresses undesirable oscillations that can lead to fluctuations in reactor temperature, catalyst circulation, product quality, and energy consumption. Improved dynamic stability can reduce process variability, facilitate tighter control, minimize off-specification production, and increase the operational flexibility of industrial FCC units. Consequently, the proposed stability-aware optimization framework provides both economic and operational benefits and offers a practical methodology that can be extended to other large-scale nonlinear chemical processes exhibiting oscillatory instabilities.

The proposed stability-aware optimal control framework provides important benefits from a green engineering perspective by enabling more efficient and sustainable operation of fluid catalytic cracking (FCC) systems. FCC units are among the largest energy-consuming operations in petroleum refining, and improvements in reactor efficiency can directly reduce energy consumption and lower greenhouse gas emissions. By avoiding Hopf bifurcation-induced oscillatory operation, the proposed approach minimizes undesirable fluctuations in reactor temperature, catalyst circulation, and reaction conditions, allowing the process to operate closer to optimal and energy-efficient regimes. The approximately 19%

improvement in cracking reaction rate achieved through Hopf-constrained optimization suggests that higher productivity can be obtained without increasing reactor size or additional energy input, thereby improving resource utilization. Furthermore, maintaining stable operating conditions can enhance catalyst effectiveness by reducing thermal excursions and minimizing conditions that accelerate catalyst deactivation and coke formation. Improved dynamic control can also contribute to more consistent product quality, potentially reducing waste associated with off-specification products and improving downstream processing efficiency. Therefore, integrating nonlinear stability analysis with optimal control provides a pathway toward greener FCC operation by simultaneously improving productivity, operational reliability, and environmental performance. The proposed framework can be further extended by integrating digital twins, artificial intelligence, and real-time process optimization tools to support the development of next-generation sustainable refining technologies.

Overall, the results demonstrate that nonlinear dynamic phenomena are not merely theoretical characteristics of FCC systems but play a direct role in determining achievable process performance. The presented Hopf-aware optimal control framework provides a systematic mechanism for simultaneously improving productivity and enhancing dynamic stability. The demonstrated increase in cracking performance, together with the suppression of oscillatory behavior, highlights the significant industrial potential of incorporating bifurcation-theoretic concepts into advanced process optimization and control methodologies.

4. Conclusion

In this work, a nonlinear dynamic and optimal control framework was developed for a fluid catalytic cracking system exhibiting complex bifurcation behavior. The proposed FCC model was analyzed using continuation and bifurcation techniques in order to investigate the influence of operating conditions on process stability and reactor performance. The obtained results demonstrated the existence of multiple steady states, a limit point bifurcation, and Hopf bifurcation induced oscillatory dynamics, confirming the strongly nonlinear nature of the FCC process.

The bifurcation analysis revealed that variations in the air-flow parameter can significantly alter the qualitative behavior of the system. In particular, the detection of a Hopf bifurcation together with a positive first Lyapunov coefficient confirmed the emergence of oscillatory dynamics through a subcritical Hopf bifurcation mechanism. Continuation of the Hopf point further demonstrated the existence of sustained limit cycle oscillations. These findings are important because oscillatory reactor-regenerator behavior is undesirable in industrial FCC operation and may lead to reduced conversion efficiency, unstable thermal behavior, increased coke formation, and operational difficulties. The presence of a limit point additionally indicated the existence of multiplicity and turning-point behavior, emphasizing the sensitivity of FCC systems to operating conditions and control actions.

An optimal control formulation was subsequently developed to maximize the cracking reaction rate while accounting for nonlinear dynamic stability. The results showed that incorporating Hopf bifurcation avoidance within the optimization problem significantly improved process performance. Without the Hopf constraint, the optimal cracking rate achieved was 6.254, whereas implementation of the Hopf-aware constraint increased the cracking rate to 7.443, corresponding to an improvement of approximately 19%. This demonstrates that avoiding unstable oscillatory operating regimes can directly enhance reactor productivity and operational efficiency.

From an industrial perspective, the proposed methodology provides a systematic strategy for operating FCC units in dynamically stable and economically favorable regions. The integration of bifurcation analysis with optimal control offers several practical advantages, including suppression of undesirable oscillations, improved process stability, enhanced catalyst utilization, and increased

operational reliability. Moreover, the framework ensures that the computed optimal solutions are not only mathematically optimal but also dynamically feasible for practical implementation.

Although the present study demonstrates the potential of bifurcation-aware optimal control for improving the performance of FCC systems, several limitations should be acknowledged. The analysis is based on a nonlinear dynamic simulation model, and the reported productivity improvement has not yet been validated using experimental measurements or industrial FCC operating data. Therefore, the results should be interpreted as demonstrating the potential benefits of incorporating dynamic stability considerations into process optimization rather than as a direct prediction of industrial performance gains. Future studies should focus on validating the proposed framework using pilot-scale experiments, industrial operating datasets, and high-fidelity FCC simulation platforms. In addition, uncertainty quantification and sensitivity analysis should be performed to evaluate the influence of kinetic parameters, catalyst properties, operating disturbances, and model uncertainties on the predicted optimal solutions and bifurcation behavior. The integration of the proposed methodology with digital twin platforms and physics-informed machine learning models represents another important research direction, enabling real-time stability monitoring and adaptive optimization under realistic plant conditions. Such developments would further establish the practical applicability of stability-aware optimal control for improving the efficiency, reliability, and sustainability of large-scale FCC operations.

Overall, this work highlights the importance of combining nonlinear dynamics, bifurcation theory, and optimal control for advanced chemical process operation. The proposed Hopf-aware optimization framework establishes a strong foundation for future studies involving artificial intelligence-assisted control, bifurcation-constrained optimization, and stability-aware operation of large-scale nonlinear industrial processes.

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APPENDIX

Tables 1 and 2 provide details on the variables and parameters.

Table 1. Variables

Symbol	Variable Name	Units
T_r	Riser reactor temperature	K
T_g	Regenerator temperature	K
C_c	Coke concentration on catalyst	kg coke/kg catalyst
O_2	Oxygen concentration in regenerator	mol/m ^{3}
F_c	Catalyst circulation rate	kg/s
F_{air}	Regenerator air flow rate	kg/s
F_f	Feed flow rate	kg/s
T_f	Feed preheat temperature	K
T_{air}	Inlet air temperature	K
C_f	Feed hydrocarbon concentration	mol/m ^{3}
R_r	Cracking reaction rate	mol/(m ^{3} ·s)
R_b	Coke combustion reaction rate	mol/(m ^{3} ·s)
V_r	Riser reactor volume	m ^{3}
V_g	Regenerator volume	m ^{3}
M_r	Effective riser mass inventory	kg
M_g	Regenerator mass inventory	kg
M_c	Catalyst inventory	kg
$F_{c,set}$	Desired catalyst circulation rate	kg/s
$O_{2,in}$	Inlet oxygen concentration	mol/m ^{3}

Table 2. Parameters

Symbol	Variable / Parameter Name	Units
C_{pf}	Feed heat capacity	J/(kg·K)
C_{pc}	Catalyst heat capacity	J/(kg·K)
C_{pg}	Regenerator heat capacity	J/(kg·K)
C_{pa}	Air heat capacity	J/(kg·K)
ΔH_r	Heat of cracking reaction	J/mol
ΔH_b	Heat of coke combustion	J/mol
k_r	Cracking reaction pre-exponential factor	s^{-1}
k_b	Coke combustion pre-exponential factor	s^{-1}
E_r	Activation energy for cracking reaction	J/mol
E_b	Activation energy for coke combustion	J/mol
R	Universal gas constant	J/(mol·K)
Y_c	Coke yield coefficient	kg coke/mol reacted feed
ν_b	Oxygen consumption coefficient	mol O_2/mol coke
τ_c	Catalyst circulation time constant	s
α_c	Thermal circulation coupling coefficient	kg/(s·K)

Tables 3 and 4 have details about the scaled variables and scaled parameters.

Table 3. Scaled Variables

Symbol	Variable / Parameter Name	Units / Meaning
θ_r	Scaled riser temperature deviation	Dimensionless
θ_g	Scaled regenerator temperature deviation	Dimensionless
c	Coke concentration on catalyst (scaled)	Dimensionless
0	Oxygen concentration (scaled)	Dimensionless
f	Scaled catalyst circulation rate	Dimensionless
u	Scaled air flow rate (bifurcation/control input)	Dimensionless
T_r	Physical riser temperature (back-scaled)	K
T_g	Physical regenerator temperature (back-scaled)	K
F_c	Catalyst circulation rate (back-scaled)	kg/s
F_{air}	Air flow rate (back-scaled)	kg/s
R_r	Cracking reaction rate	mol/(m³·s)
R_b	Coke combustion rate	mol/(m³·s)
T_f	Feed temperature (fixed input)	K
T_{air}	Air inlet temperature (fixed input)	K
F_f	Feed flow rate (fixed input)	kg/s
$O_{2,in}$	Inlet oxygen concentration	mol/m³
M_r	Riser mass inventory	kg
M_g	Regenerator mass inventory	kg
M_c	Catalyst inventory	kg

Table 4. Scaled Parameters

Parameter	Parameter Name	Units / Role
C_{pf}	Feed heat capacity	J/(kg·K)
C_{pc}	Catalyst heat capacity	J/(kg·K)
C_{pg}	Regenerator heat capacity	J/(kg·K)
C_{pa}	Air heat capacity	J/(kg·K)
ΔH_r	Heat of cracking reaction	J/mol
ΔH_b	Heat of coke combustion	J/mol
k_r	Cracking reaction pre-exponential factor	s⁻¹
k_b	Coke combustion pre-exponential factor	s⁻¹
E_r	Activation energy (cracking)	J/mol
E_b	Activation energy (combustion)	J/mol
R	Universal gas constant	J/(mol·K)
Y_c	Coke yield coefficient	kg coke/mol feed reacted
ν	O_2 stoichiometric coefficient	mol O_2/mol coke
τ_c	Catalyst circulation time constant	s
α_c	Thermal coupling coefficient	kg/(s·K)
V_r	Riser reactor volume	m³
V_g	Regenerator volume	m³
M_r	Riser mass inventory	kg
M_g	Regenerator mass inventory	kg
M_c	Catalyst inventory	kg
F_f	Feed flow rate (fixed input)	kg/s
T_f	Feed temperature (fixed input)	K
T_{air}	Air inlet temperature	K
$O_{2,in}$	Inlet oxygen concentration	mol/m³
scaling constants	700, 750, 100, 10, 5	reference scaling values for nondimensionalization