

Article

Optimization of the Combustion Kinetic Mechanism and Investigation of Combustion Characteristics in NH₃/CH₄ Co-Firing

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Abstract

Existing NH₃/CH₄ combustion reaction mechanisms still exhibit a pronounced trade-off between predictive accuracy and computational efficiency. It is difficult to guarantee global optimality, which limits their application in gas turbine combustion simulations. The objective of this study was to introduce machine learning methods into the parameter optimization process of combustion reaction mechanisms and to construct an optimized mechanism (Bys-BP Mech) with both high accuracy and high computational efficiency. First, a reduced mechanism was obtained through mechanism coupling and the DRGEP method. Subsequently, the pre-exponential factors and activation energies of three key reactions were optimized based on sensitivity analysis. An artificial neural network was used to construct the model, and cross-validation combined with Bayesian optimization was employed to achieve automatic hyperparameter optimization. Validation results showed that the optimized Bys-BP Mech achieved an average relative error of 4.56% for LBV, and the average relative error of IDT decreased to 17.16%. CFD simulations indicated that the minimum prediction error of NO emissions was 3.74% when the CH₄ co-firing ratio ranged from 40% to 70%. This mechanism addressed the limitations of existing mechanisms in combustor-scale validation under variable operating conditions and reduced the computational time of combustion simulations by half.

Keywords: NH₃/CH₄ co-firing; mechanism optimization; artificial neural network; laminar burning velocity; ignition delay times; sensitivity analysis



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1. Introduction

The combustion of fossil fuels such as methane (CH₄) is one of the main sources of carbon dioxide (CO₂) emissions [1]. Combustion technologies involving CH₄ co-firing with zero-carbon fuels such as hydrogen (H₂) or ammonia (NH₃) have attracted considerable attention owing to their extensive use in the power sector [2,3]. H₂ poses safety risks during storage and transportation, whereas NH₃ is more suitable for large-scale transportation and utilization [4]. However, its high toxicity can seriously threaten the ecological environment and human health after leakage. Therefore, its safety risks need to be carefully assessed while promoting NH₃ as a low-carbon fuel. In addition, NH₃ has a narrow flammability range and a low flame temperature, and NO_x emissions may be generated during combustion [5–7]. These challenges can be effectively mitigated by co-firing NH₃ with CH₄ [8]. However, detailed chemical mechanisms usually contain hundreds to thousands of species and reactions, which

increases the difficulty of interpretation and the computational cost [9]. Therefore, constructing a compact and reliable NH_3/CH_4 combustion reaction mechanism is of great significance.

Regarding studies on NH_3/CH_4 co-firing reaction mechanisms, the mechanism proposed by Okafor et al. showed good agreement with experimental laminar burning velocity (LBV) data, but exhibited relatively low accuracy in predicting ignition delay time (IDT) [10,11]. Hou et al. [12] developed a new mechanism based on the Okafor-reduce mechanism [10], which could accurately calculate the LBV of NH_3/CH_4 over a wide blending-ratio range, but IDT was not validated. Han et al. [13] developed a mechanism containing 85 species and 475 reactions for NH_3 and syngas, which could reasonably predict LBV and IDT, but overpredicted LBV and underestimated IDT under certain operating conditions. Zhu et al. [14] developed a reduced mechanism containing 53 species and 353 reactions for NH_3/CH_4 co-firing, which can satisfactorily predict LBV over wide equivalence-ratio and pressure ranges, but the discussion of the combustion characteristics of NH_3/CH_4 binary mixtures remains relatively limited. Liao et al. [15] developed a mechanism containing 39 species and 325 reactions, which can reproduce the LBV of NH_3/CH_4 co-firing well under oxygen-lean conditions, but its LBV prediction error gradually increases as the equivalence ratio increases. These studies indicate that the mechanisms constructed in the above investigations still struggle to accurately predict both LBV and IDT, and systematic validation under wide operating conditions, such as different pressures and variable heat loads, remains insufficient.

With the rapid development of machine learning, robust data-driven models have been developed and applied. Roy et al. [16] simplified a detailed $\text{CH}_4/\text{NH}_3/\text{H}_2$ mechanism based on an artificial neural network (ANN), yielding reduced mechanisms with 48 species (using IDT as the target parameter) and 59 species (using LBV as the target parameter), respectively. However, the mechanism using IDT as the target parameter showed large deviations in LBV prediction. Mao et al. [17] employed three ANN models to predict NO_x emissions during NH_3/H_2 combustion, but experimental validation was lacking, and the generalization capability under practical combustion conditions requires further examination. Huang et al. [18] optimized the kinetic parameters of five key elementary reactions using ANN and proposed an NH_3/CH_4 combustion reaction mechanism containing 23 species and 73 reactions, which reduced the prediction errors of IDT, LBV, and NO emissions under atmospheric pressure. However, it was limited to a single atmospheric-pressure condition, and its generalization capability under different pressure conditions remains to be assessed. In addition, Liu et al. [19] adopted Bayesian optimization to efficiently search for optimal experimental conditions, thereby reducing model prediction errors and parameter uncertainty. However, that study mainly focused on the optimal selection of experimental conditions rather than the calibration of mechanism parameters. Table 1 lists recent progress in mechanism reduction and optimization, indicating that systematic validation of the generalization capability of optimized mechanisms under variable operating conditions remains insufficient. Therefore, ANN and Bayesian optimization were synergistically applied in this study to the parameter calibration of the NH_3/CH_4 combustion mechanism to improve its predictive reliability.

To further validate the combustion characteristics of mechanisms under different operating conditions, Xi et al. [20] numerically investigated NH_3/Air and $\text{CH}_4/\text{H}_2/\text{Air}$ co-firing in a radially staged combustor using Computational Fluid Dynamics (CFD). They revealed the effects of the H_2 blending ratio on the flow field, temperature field, and NO formation pathways, but three-dimensional flow details could not be fully captured, and NO prediction showed large deviations under fuel-rich conditions. Liu et al. [21] numerically simulated the combustion and emission characteristics of NH_3/CH_4 axially staged combustion under premixed and non-premixed modes using CFD. They elucidated

the influence mechanisms of the staged-air ratio and injection height on NO and CO formation as well as the optimal operating conditions, but their applicability to practical high-pressure gas turbine conditions requires further validation. Tu et al. [22] investigated the combustion and emission characteristics of NH_3/CH_4 premixed swirling flames under air-staged and non-staged modes through experiments and CFD. They maintained high combustion efficiency while reducing NO emissions by optimizing parameters such as the staged-air ratio and injection height, but large deviations occurred in CO emission prediction. Qiu et al. [23] conducted high-temperature and high-pressure experiments and large-eddy simulations on the variable-load process of a radially staged combustor. They expanded the stable operating boundary of combustion while satisfying NO_x and CO emission requirements, providing engineering guidance for variable-load operation under peak-shaving conditions. The above studies mainly focused on combustion characteristics and emission patterns under fixed operating conditions, whereas CFD simulations under different heat loads remain relatively limited.

In summary, existing NH_3/CH_4 combustion reaction mechanisms remain insufficient for accurately predicting both LBV and IDT, and systematic validation under different heat load conditions is still lacking. Therefore, ANN, cross-validation, and Bayesian optimization were combined to optimize key kinetic parameters, and an optimized mechanism applicable to NH_3/CH_4 combustion (Bys-BP Mech) was constructed in this study. On this basis, the accuracy of this mechanism in predicting LBV and IDT was validated, and the effects of different heat loads on the temperature field, flow-field distribution, and NO formation characteristics were analyzed through CFD simulations in this study. This machine learning method provides a data-driven pathway for the construction and optimization of combustion reaction mechanisms and can offer new technical insights and references for the intelligent development of combustion kinetic modeling.

Table 1. Summary of recent studies on NH_3/CH_4 co-firing mechanisms.

Mechanism	Fuel	Species/Reaction	Method	Validation	Accuracy
Okafor 2019 [10]	NH_3/CH_4	42/130	DRGEP, SA	LBV	within exp. uncertainty
Hou 2026 [12]	NH_3/CH_4	42/130	SA	LBV	LBV improved
Han 2023 [13]	NH_3/H_2	85/475	SA	LBV, IDT	LBV error 0.89 cm/s, IDT improved
Zhu 2024 [14]	$\text{NH}_3/\text{CH}_4/\text{H}_2/\text{CO}$	53/353	DRG, DRGEP, CSP	LBV, IDT	Excellent agreement
Liao 2025 [15]	NH_3/CH_4	39/325	DRGEP, DRGEPsA, FSSA	LBV, IDT	LBV max error 7.3%, IDT error < 1%
Roy 2026 [16]	$\text{NH}_3/\text{CH}_4/\text{H}_2$	48/370	ANN, Sobol-GSA	LBV, IDT, CFD simulation	Excellent agreement
Huang 2025 [18]	NH_3/CH_4	23/73	DRGEP, CSP, ANN	LBV, IDT, CFD simulation	LBV error 5.6%, IDT error: 3%, NO error reduced by 30%
Wang 2022 [24]	NH_3/CH_4	91/444	SA	LBV, IDT	Excellent agreement

2. Research Methods and Conditions

2.1. Construction and Optimization of the Combustion Mechanism

The overall methodology adopted in this study is shown in Figure 1, mainly including mechanism coupling, reduction, optimization, and validation processes. The classical combustion reaction models Okafor [6], Huang [18], Wang [24], and GRI3.0 [25], which are applicable over wide operating ranges, were selected in this study. These mechanisms exhibit high prediction accuracy for LBV and IDT and can serve as reliable benchmarks for

subsequent mechanism coupling and data-driven optimization. IDT and LBV simulations were performed using ANSYS Chemkin 2021 R2 and compared with relevant experimental data. Finally, the Huang and Okafor mechanisms were selected for coupling.

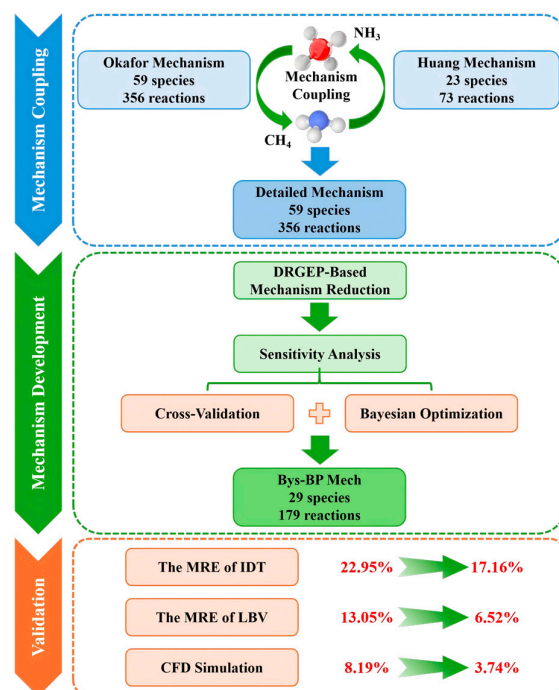


Figure 1. Overall workflow for the development and validation of the combustion mechanism based on machine learning.

The LBV was predicted using the laminar premixed reactor model and compared with the experimental values reported by Han et al. [26]. The experimental conditions of Han et al. were an equivalence ratio of $\Phi = 0.7 \sim 1.6$, a CH_4 blending ratio of $X_{\text{CH}_4} = 20 \sim 60\%$, a burner ambient temperature of 413 K, a fuel inlet temperature of 298 K, and a pressure of 1 atm. The simulated IDT values were obtained using the homogeneous reactor model and compared with the experimental data reported by Shu et al. [27] and Xiao et al. [28]. The rapid compression machine used by Shu et al. and Xiao et al. had a volume of 10 L, and adiabatic, homogeneous, and constrained-volume assumptions were applied. The shock tube volume was 0.0746 m^3 , and the specific conditions are listed in Table 2.

Table 2. IDT experimental conditions of Shu et al. [27] and Xiao et al. [28].

Case		X_{CH_4}	Pressure (atm)	Equivalence Ratio
Shu	Case1	20%	19.74	0.5
	Case2	10%	19.74	2
Xiao	Case3	40%	5	0.5
	Case4	40%	5	2

The Mechanism Utilities module in Chemkin was selected to couple the Huang and Okafor mechanisms. The Okafor mechanism, which showed higher predictive accuracy for IDT, was used as the primary reaction mechanism model, and the Huang mechanism, which exhibited higher predictive accuracy for LBV, was used as the secondary reaction mechanism model. The kinetic parameters in the primary reaction mechanism were preferentially adopted when identical elementary reactions and rate constants were encountered. The Okafor mechanism contained 59 species and 356 elementary reactions, while the Huang mech-

anism comprised 65 species and 466 elementary reactions. The coupled detailed mechanism (Detailed Mech) for NH_3/CH_4 co-firing contained 65 species and 471 elementary reactions.

Mechanism reduction was performed using the Directed Relation Graph with Error Propagation (DRGEP) method, which accounted for the effect of error propagation in the relation graph on the evaluation of species dependence and corrected the coefficients of direct interactions among species in the mechanism, as shown in Equations (1)–(3):

$$r_{AB} = \frac{\left| \sum_{i=1}^I (v_{A,i} \omega_i \delta_B^i) \right|}{\max(P_A, C_A)} \quad (1)$$

$$P_A = \sum_{i=1}^I \max(0, v_{A,i} \omega_i) \quad (2)$$

$$C_A = \sum_{i=1}^I \max(0, -v_{A,i} \omega_i) \quad (3)$$

where r_{AB} is the coupling coefficient between species A and B, i is the i th reaction, $v_{A,i}$ is the stoichiometric coefficient of species A in the i th reaction, ω_i is the net reaction rate of the i th reaction ($\text{mol}/\text{s}\cdot\text{m}^3$), and I is the total number of reactions. The term δ_B^i equals 1 if the i th reaction involves species B, and 0 otherwise. P_A and C_A represent the production rate and consumption rate of species A, respectively [18].

The key innovation of the DRGEP method lies in its consideration of not only direct coupling relationships but also the indirect propagation effects of errors along reaction pathways. Along a specific path p , the dependence of species A on species B is characterized by the path coupling coefficient $r_{AB,p}$, which is expressed by Equation (4):

$$r_{AB,p} = \prod_{j=1}^{n-1} r_{S_j S_{j+1}} \quad (4)$$

where n is the number of species traversed from A to B along path p , and S_j is an intermediate species on the pathway [15]. The overall dependence of species A on species B, R_{AB} , is defined as the maximum coupling coefficient among all possible pathways, as shown in Equation (5):

$$R_{AB} = \max_{\text{all path } p} (r_{AB,p}) \quad (5)$$

The species selection criterion of DRGEP is defined as follows: if at least one pathway exists from target species A to species B and its R_{AB} value is greater than the prescribed threshold ε , this species must be retained in the reduced mechanism. Conversely, if the R_{AB} values of a given species B relative to the target species are lower than ε along all possible pathways, this species is considered to have a minor influence on the target parameters and can be removed [15].

The reduction process was performed under combustor operating conditions, with operating ranges of $P = 2\sim 5$ atm and $T = 1100\sim 1800$ K. IDT, CO, and NO concentrations were selected as the target parameters. CO and NO are key intermediate products during NH_3/CH_4 combustion, and their reaction pathways affect exhaust emissions [27]. CH_4 , CO, CO_2 , H_2O , N_2 , NH_3 , NO, and O_2 were first selected as the initially retained species, because CO, CO_2 , H_2O , N_2 , and NO are the most important products and nitrogen oxide precursors during combustion, and their concentrations and reaction pathways directly affect the predictive accuracy of IDT and NO emissions [14]. The dependence coefficient R_{AB} of each species on the target species was calculated using Equation (5), and the key species that directly or indirectly influenced the target parameters were identified. On this basis, a relative error threshold of $\varepsilon = 30\%$ was specified to ensure a reasonable balance between prediction accuracy and computational scale after reduction, and all species with

$R_{AB} < \varepsilon$ and their associated reactions were removed [18]. Finally, a reduced mechanism (Reduced Mech) consisting of 29 species and 179 elementary reaction steps was obtained.

To determine the influence intensity of key reactions on combustion characteristics, the effects of different CH₄ blending ratios, pressures, and temperatures on IDT were investigated based on sensitivity analysis in this study. The sensitivity coefficient was defined by Equation (6):

$$S = \frac{\tau(k_i) - \tau(k_{2i})}{\tau(k_{2i})} \quad (6)$$

where k_i is the rate constant of the i th reaction, $\tau(k_i)$ is the IDT when the reaction rate remains unchanged, and $\tau(k_{2i})$ is the IDT when the rate constant of the i th reaction is doubled. A positive sensitivity coefficient indicates that IDT increases when the reaction rate is doubled, thereby inhibiting the fuel ignition process, whereas a negative value promotes ignition [18].

In this study, a comprehensive analysis identified the top 10 elementary reactions exerting the greatest influence on IDT in Reduced Mech, as listed in Table 3. Four elementary reactions associated with CH₃ were included among them. Ignition occurrence depended on the rate of H-abstraction, and CH₄ blending supplied abundant H* and OH* during the reaction process, thereby intensifying the ignition process.

Table 3. Top 10 elementary reactions with significant effects on IDT under different operating conditions.

Reaction	Reaction Equation	A ((cm ³ /mol) ⁿ⁻¹ /s)	b	Ea (cal/mol)
R23	H + O ₂ <=> O + OH	1.04×10^{14}	0.00	15,286.00
R38	H + CH ₂ O(+M) <=> CH ₃ O(+M)	5.40×10^{11}	0.45	2600.00
R57	OH + CH ₄ <=> CH ₃ + H ₂ O	1.00×10^8	1.60	3120.00
R65	HO ₂ + CH ₃ <=> OH + CH ₃ O	3.78×10^{13}	0.00	0.00
R79	CH ₃ + O ₂ <=> O + CH ₃ O	3.56×10^{13}	0.00	30,480.00
R80	CH ₃ + O ₂ <=> OH + CH ₂ O	2.31×10^{12}	0.00	20,315.00
R87	CH ₃ O + O ₂ <=> HO ₂ + CH ₂ O	4.28×10^{-13}	7.60	−3530.00
R112	NH ₂ + HO ₂ <=> NH ₃ + O ₂	9.20×10^5	1.94	−1152.00
R113	2NH ₂ <=> NH ₃ + NH	5.00×10^{13}	0.00	10,000.00
R137	NH ₃ + OH <=> NH ₂ + H ₂ O	2.00×10^6	2.04	566.00

Sensitivity analysis of Reduced Mech showed that the CH₄ co-firing ratio, pressure, and temperature significantly affected the key elementary reactions governing IDT. As the CH₄ proportion increased, the inhibiting effects of R57 and R23 on IDT weakened, with the sensitivity coefficients decreasing from 0.400 and 0.358 to 0.160 and 0.229, respectively. Meanwhile, the CH₃ concentration increased, making R79 and R87 the dominant reactions. As the pressure increased, the promoting effect of R87 was enhanced, with the coefficient decreasing from −0.26 to −0.28, whereas the inhibiting effects of R23 and R57 were strengthened, with the coefficients increasing to 0.30 and 0.22, respectively.

Considering all operating conditions, the reactions exerting substantial effects on IDT included R23, R57, R79, R87, R112, R65, and R64. In addition, the reactions with the highest sensitivities to CO and NO concentrations were R23 and R117, respectively, with an inhibition coefficient of 0.34 for CO by R23 and an inhibition coefficient of 0.48 for NO by R117. Accordingly, the pre-exponential factors (A) and activation energies (Ea) of R23, R57, and R79 were selected as optimization parameters, while the temperature exponents b were kept unchanged in this study. This was because the sensitivity coefficients of R23, R57, and R79 reached 0.400, 0.358, and 0.280, respectively, and these reactions maintained significant dominance under different CH₄ blending ratios, pressures, and temperatures. If more reactions were optimized, the computational cost would increase exponentially, whereas

the marginal improvement in prediction accuracy would be limited. This strategy was consistent with the ANN-based kinetic optimization study conducted by Huang et al. [18].

Because ANN can accurately model the intrinsic patterns of training data and possesses strong nonlinear modeling capability, feature adaptivity, and advantages in effectively capturing high-order interactions, an initial neural network model (BP Model) was constructed using ANN in this study to support the optimization of the reduced reaction mechanism. Figure 2 shows the architecture of the initial BP Model, which contained two hidden layers with eight neurons in each layer.

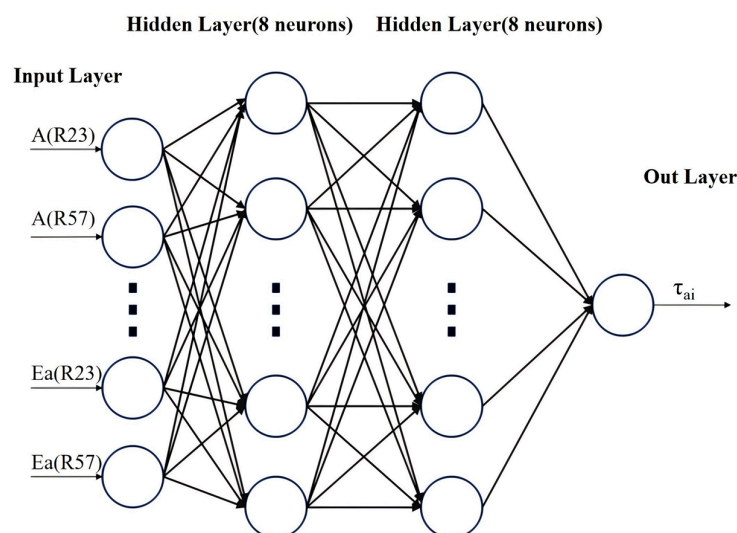


Figure 2. Structure of the initial neural network.

The six input parameters of the initial BP Model were A and E_a for three elementary reactions (R23, R57, and R79), and the output parameter was IDT. The input parameters were randomly generated within the specified ranges of A and E_a , as shown in Table 4. A total of 6000 groups of data randomly generated within the range of each parameter were used as the input parameters of the initial BP Model. The obtained 6000 groups of A and E_a were then imported into the Chemkin zero-dimensional homogeneous reactor model for numerical simulations, yielding 6000 groups of IDT. Before training, all input and output parameters were normalized [18], as shown in Equation (7):

$$P_{nor} = \frac{P - P_{min}}{P_{max} - P_{min}} \quad (7)$$

where P_{max} represents the maximum value among all parameters, and P_{min} represents the minimum value among all parameters.

Table 4. Randomly generated ranges of A and E_a for the selected elementary reactions.

Reaction	A_{min} ((cm ³ /mol) ⁿ⁻¹ /s)	A_{max} ((cm ³ /mol) ⁿ⁻¹ /s)	$E_{a_{min}}$ (cal/mol)	$E_{a_{max}}$ (cal/mol)
R23	1.04×10^{13}	1.04×10^{15}	12,000.00	18,000.00
R57	1.00×10^7	1.00×10^9	2100.00	4100.00
R79	3.56×10^{12}	3.56×10^{14}	28,000.00	35,000.00

The dataset was divided into 80% training set and 20% test set. The coefficients of determination (R^2) of the initial model were 0.99749 for the training set and 0.99697 for the test set, respectively, as shown in Figure 3. The coefficient of determination for the test set was only 0.00052 lower than that for the training set, indicating no overfitting and

confirming the predictive reliability of the model for new data. The model could effectively capture the nonlinear mapping between the inputs and IDT. To further improve the linear correlation of the predictions, 5-fold cross-validation and Bayesian optimization were employed for model optimization, and whether the model architecture or hyperparameters needed to be adjusted was evaluated. The cross-validation loss and Mean Squared Error (MSE) are defined in Equations (8) and (9):

$$CV\ Loss = \frac{1}{K} \sum_{i=1}^K MSE \quad (8)$$

$$MSE = \frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2 \quad (9)$$

where $CV\ Loss$ is the cross-validation loss, K is the number of folds, N is the total number of samples, y_i is the true value of the i th sample, and $\hat{y}_i$ is the predicted value of the i th sample [29].

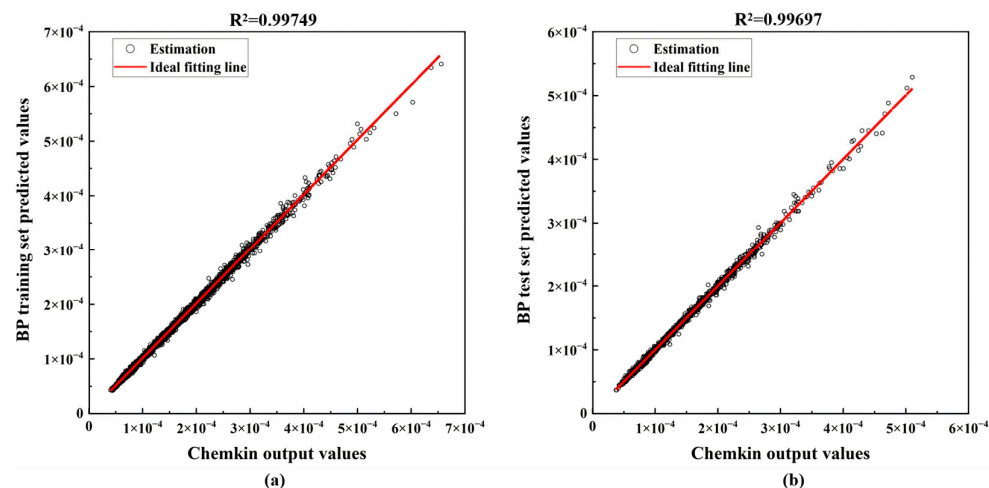


Figure 3. Fitting performance of the initial BP Model for the (a) training set and (b) test set.

After cross-validation, the number of neurons was adjusted to 16 + 8, and the validation loss was 0.0023383. The relatively high validation loss indicated that Bayesian optimization was required for subsequent hyperparameter optimization of the model. The core concept of Bayesian optimization is to regard the mapping relationship between hyperparameters and model performance as an unknown function, construct a probabilistic surrogate model of this function using a Gaussian process, and adaptively select the next evaluation point in the hyperparameter space through an acquisition function, thereby approaching the global optimum within fewer iterations. During the optimization process, minimization of the 5-fold cross-validation loss was used as the objective function, and the maximum number of iterations was set to 50.

After Bayesian optimization, the model architecture was changed to 16 + 12 neurons, and the activation function was expanded from a single ReLU to a combination of ReLU and Tanh [30]. The regularization coefficient was reduced from 5×10^{-3} to 9.9841×10^{-8} , enabling the model to fit the training data more flexibly. R^2 increased to 0.99989 for the training set and 0.99980 for the test set, as shown in Figure 4.

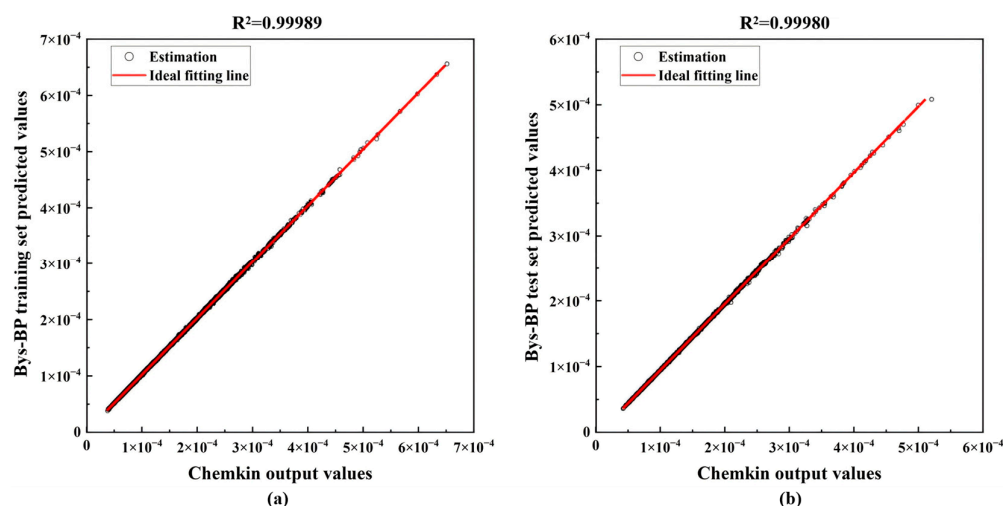


Figure 4. Fitting performance of the Bys-BP Model on the (a) training set and (b) validation set.

After optimization, the mean relative error (4.56%) was used as the evaluation metric, and this value was lower than the experimental measurement uncertainty of 5%. The optimized model showed consistent performance in terms of the mean absolute error (MAE), root mean squared error (RMSE), and R^2 , with reduced errors. The comparison of performance metrics before and after model optimization is presented in Table 5.

Table 5. Comparison of performance indicators before and after model optimization.

Metrics	Data Set	BP Model	Bys-BP Model	Amplitude of Variation
R^2	Training set	0.99749	0.99989	0.24%
	Test set	0.99697	0.99980	0.28%
MAE	Training set	2.73×10^{-6}	5.60×10^{-7}	−78.49%
	Test set	2.94×10^{-6}	6.70×10^{-7}	−77.21%
RMSE	Training set	3.83×10^{-6}	8.10×10^{-7}	−78.85%
	Test set	4.18×10^{-6}	1.07×10^{-6}	−74.40%

Finally, the trained Bys-BP Model was applied to elementary reaction parameter optimization. The reference IDT values were calculated using Detailed Mech under identical thermodynamic conditions. Subsequently, 30,000 sets of parameter combinations were randomly generated, and the IDT was predicted using the model. Parameters with errors relative to the reference values of less than 10^{-6} were screened, as shown in Table 6. These parameters were incorporated into the reduced mechanism, yielding the optimized Bys-BP Mech.

Table 6. Optimized values of A and E_a for the three elementary reactions.

Reaction	Reaction Equation	$A \text{ ((cm}^3/\text{mol)}^{n-1}/\text{s)}$	$E_a \text{ (cal/mol)}$
R23	$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$	2.2012×10^{14}	17,657.00
R57	$\text{OH} + \text{CH}_4 \rightleftharpoons \text{CH}_3 + \text{H}_2\text{O}$	8.4999×10^8	3296.46
R79	$\text{CH}_3 + \text{O}_2 \rightleftharpoons \text{O} + \text{CH}_3\text{O}$	2.9983×10^{13}	33,368.50

It should be noted that the parameters optimized using ANN may deviate from physically meaningful true values. Therefore, cross-validation and Bayesian optimization were adopted to avoid overfitting and enhance the generalization capability of the ANN model [16] in this study. Meanwhile, the optimized Arrhenius parameters listed in Table 6 were compared with data from the NIST Chemical Kinetics Database. The results showed

that the A and E_a energies of the three reactions were all within reasonable ranges of experimental uncertainty [31]. In addition, the LBV and IDT predicted by the optimized Bys-BP Mech were extensively validated against independent experimental data, and the prediction errors remained consistently low, indicating that the uncertainty introduced by ANN optimization was well controlled.

2.2. Construction of the Geometric Model and Operating Conditions

To evaluate the performance of Bys-BP Mech in CFD simulations, numerical simulations of the temperature field, flow field, and NO emission characteristics of a gas turbine were conducted under different heat loads using ANSYS Fluent 2021 R2 in this study. The combustor geometry was based on the premixed swirl flame configuration reported by Tu et al. [22]. The three-dimensional solid model was constructed using SolidWorks 2022 and then imported into ANSYS SpaceClaim for volume extraction, yielding the fluid domain containing the combustor and combustion chamber, as shown in Figure 5.

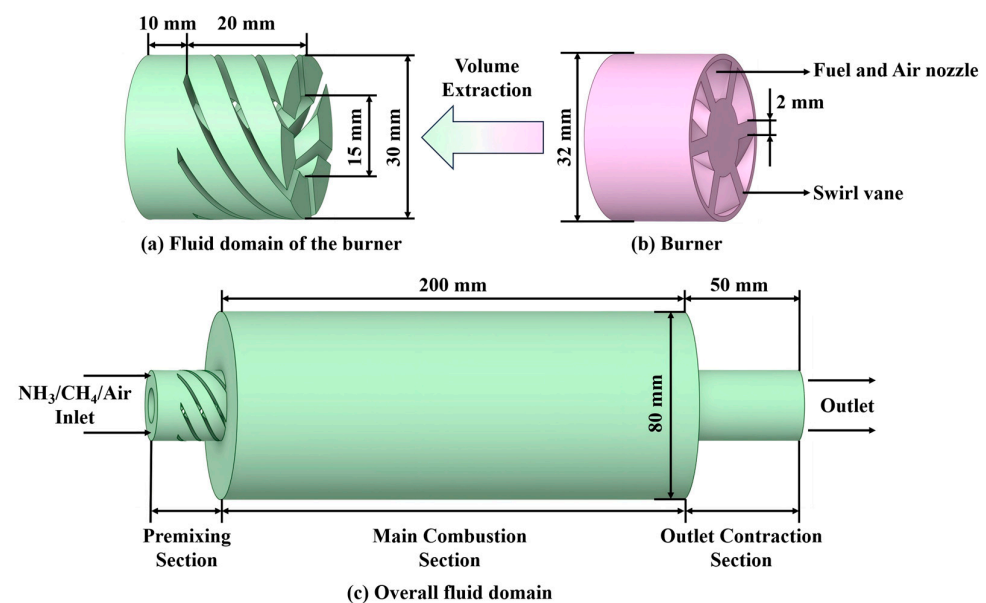


Figure 5. NH_3/CH_4 premixed swirl flame model: (a) Fluid domain of the burner, (b) Burner, and (c) Overall computational domain.

Mesh generation was performed in ANSYS Fluent Meshing using a hexahedral-dominant hybrid meshing strategy. The computational domain included the fuel-air nozzle, combustion chamber, and chimney. Since chemical reactions mainly occurred near the nozzle outlet, local mesh refinement was applied in this region, as shown in Figure 6a. To assess mesh independence, four mesh densities of 0.20 million, 0.39 million, 0.49 million, and 0.67 million cells were generated, respectively. Figure 6b presents the velocity and temperature distributions along the axial centerline of the combustion chamber. Significant discrepancies were observed among the results when the mesh size was below 0.39 million cells. The profile curves became essentially consistent when the mesh size reached 0.49 million cells or above. Considering both prediction accuracy and computational cost, the 0.49 million-cell mesh was finally adopted for subsequent simulations in this study.

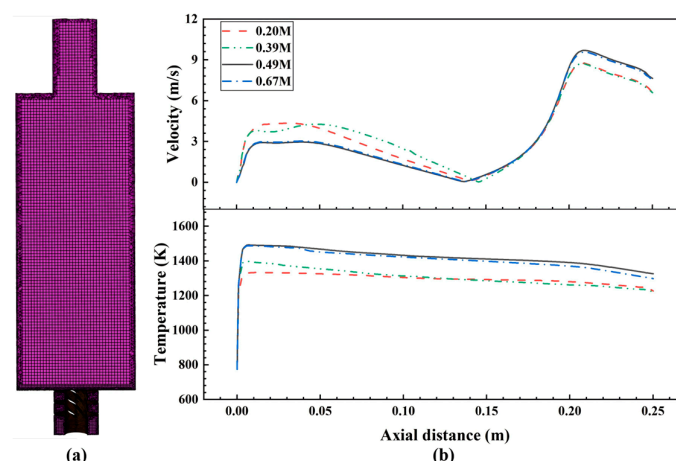


Figure 6. (a) Computational domain and mesh generation. (b) Comparison of velocity and temperature along the axial centerline of the combustion chamber under different mesh densities.

The combustor was operated at a fixed fuel power of 3 kW under ambient pressure. The combustor wall temperature was 773 K, the inlet air temperature was 298 K, the CH_4 blending ratio in the fuel was 50%, the equivalence ratio was 0.85, the swirler vane angle was 45° , and the swirl number was 0.78. To eliminate the effect of oxygen concentration differences, the NO emission data were corrected to 6% O_2 [32]. The numerical model was solved using the Realizable k - ε turbulence model, which can provide reliable solutions for combustion problems [21,33]. The chemical reactions defined in the system were numerically described using the species transport model, and the turbulence–chemistry interaction was treated using the Eddy Dissipation Concept (EDC) model. The EDC model can couple detailed chemical reaction mechanisms in the calculation of the mean reaction rate and assumes that chemical reactions occur only within the fine structures of turbulent eddies that reach the Kolmogorov scale. Their length scale (γ^*) and time scale (τ^*) are estimated by Equations (10) and (11), respectively:

$$\gamma^* = C_\gamma \left(\frac{\nu \varepsilon}{k^2} \right)^{\frac{1}{4}} \quad (10)$$

$$\tau^* = C_\tau \left(\frac{\nu}{\varepsilon} \right)^{\frac{1}{2}} \quad (11)$$

where the volume fraction constant (C_γ) and the time-scale constant (C_τ) were retained at the default values in Fluent (2.1377 and 0.4083, respectively).

The fine structures were treated as perfectly stirred reactors (PSR), within which chemical reactions proceeded at finite rates. The mass fraction of each species in the fine structures, Y_i^* , was obtained by solving Bys-BP Mech. The mean reaction rate was calculated using Equation (12):

$$R_i = \frac{\rho(\gamma^*)^2}{\tau^* [1 - (\gamma^*)^3]} (Y_i^* - Y_i) \quad (12)$$

where R_i is the mean reaction rate of species i , ρ is the fluid density, Y_i^* is the mass fraction of species i in the fine structures, and Y_i is the mean mass fraction of species i in the surrounding fluid [34]. This reaction rate was coupled into the species transport equations as a source term, thereby enabling two-way coupling between the detailed chemical reaction mechanism and the turbulent flow field. In addition, to improve the prediction accuracy of radiative heat transfer, the Discrete Ordinates (DO) radiation model was adopted in combination with the Weighted-Sum-of-Gray-Gases model (WSGG). This

model assumes that the total gas-phase emissivity is a function of temperature and partial pressure. The boundary conditions were specified as velocity inlet and pressure outlet. The detailed values of the simulation conditions under different operating conditions are listed in Table 7.

Table 7. Operating parameters.

Case	Heat Load (%)	Inlet Velocity (m/s)
1	100	2.160
2	90	1.945
3	80	1.726
4	70	1.511
5	60	1.314
6	50	1.079

3. Results and Discussion

3.1. Validation of the Optimized Mechanism

Figure 7 shows the LBV prediction results of the three mechanisms at different CH_4 blending ratios. Overall, LBV first increases and then decreases with increasing equivalence ratio, reaching its maximum at an equivalence ratio slightly above 1.0. This is because the fuel-to-oxidizer ratio approaches the stoichiometric condition, which increases the flame temperature. Meanwhile, the concentrations of radicals such as H, O, and OH also increase, thereby enhancing LBV [35]. However, as the equivalence ratio further increases, the relative deficiency of oxygen leads to a decrease in flame temperature. At the same time, the radical concentrations decline, causing LBV to decrease accordingly.

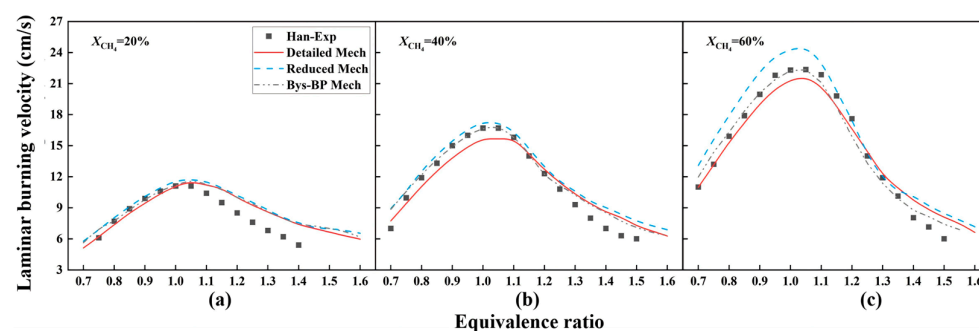


Figure 7. LBV predictions of the three mechanisms under different CH_4 co-firing ratios and equivalence ratios: (a) $X_{\text{CH}_4} = 20\%$; (b) $X_{\text{CH}_4} = 40\%$; (c) $X_{\text{CH}_4} = 60\%$.

The peak LBV differed significantly under different CH_4 blending ratios. As the CH_4 blending ratio increases, the contribution of hydrocarbon chemistry becomes more pronounced, leading to a marked increase in the peak LBV and maintaining relatively high LBV values over a broader equivalence-ratio range [35]. At CH_4 blending ratios of 20%, 40%, and 60%, the average relative errors between the LBV predictions of Bys-BP Mech and Detailed Mech were 1.72%, 5.04%, and 6.91%, respectively, with an overall average relative error of 4.56%. Therefore, the ANN-optimized mechanism can compensate for the prediction errors caused by the reduction in species composition and elementary reactions.

Figure 8 shows the IDT prediction results of the three mechanisms under different pressures and equivalence ratios. As shown in Figure 8a,b, IDT decreases with increasing pressure. The average IDT at 5 atm was 60% of that at 2 atm, and the average relative errors between the IDT predictions of the three mechanisms and the experimental values reported by Xiao et al. were relatively small. As shown in Figure 8c,d, increasing the equivalence ratio does not exert a substantial effect on IDT at pressures of 2 atm and 5 atm because the

ignition-promoting effect of CH_4 addition counterbalances the influence of NH_3 addition on IDT. However, the average relative errors between the IDT predictions of the three mechanisms and the experimental values reported by Xiao et al. increased markedly compared with those at $\Phi = 0.5$. This is because the complexity of reaction pathways increases significantly with increasing equivalence ratio, and their relative importance also changes, thereby amplifying the prediction deviations [28].

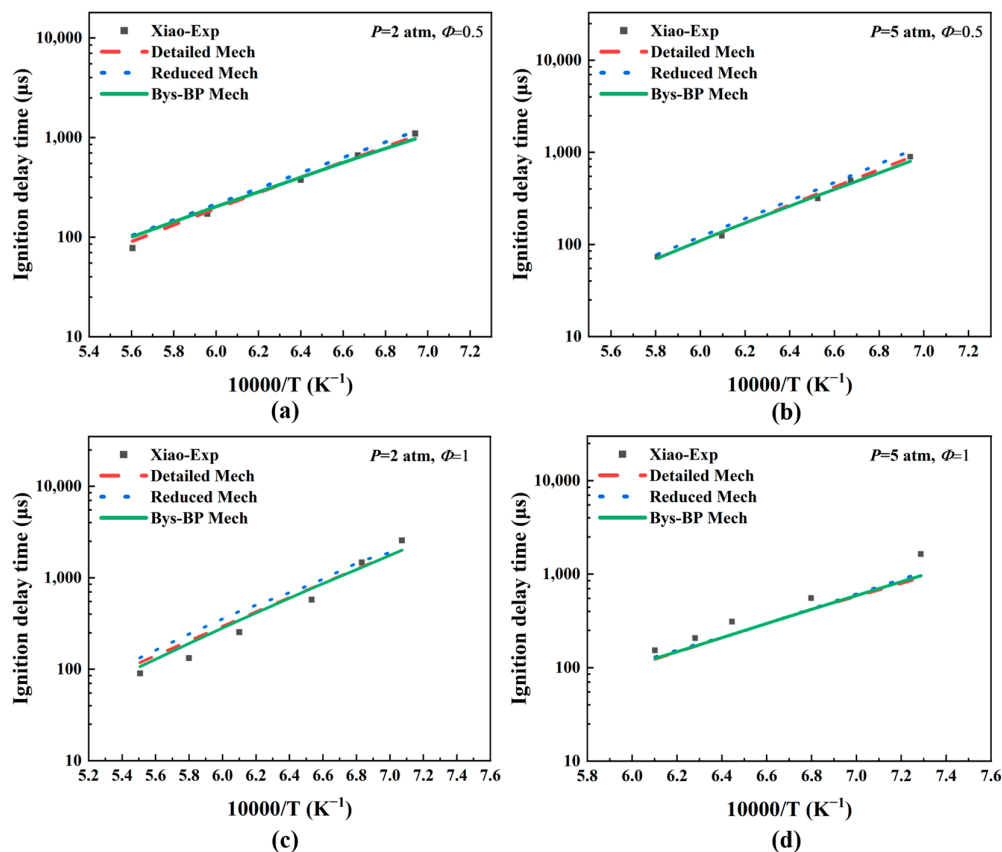


Figure 8. IDT predictions of the three mechanisms under different pressure and equivalence-ratio conditions: (a) $P = 2$ atm, $\Phi = 0.5$; (b) $P = 5$ atm, $\Phi = 0.5$; (c) $P = 2$ atm, $\Phi = 1$; (d) $P = 5$ atm, $\Phi = 1$.

Figure 9 shows the average relative errors between the simulated and experimental values of IDT under different pressures and LBV under different CH_4 blending ratios for the three mechanisms. As shown in Figure 9a, under the pressure condition of 2 atm, the average relative errors of the IDT predictions obtained using Reduced Mech, Detailed Mech, and Bys-BP Mech were 36%, 23.54%, and 22.95%, respectively. This is because an increased degree of mechanism reduction inevitably increases the prediction error of IDT. In addition, IDT is sensitive to pressure. Under the low-pressure condition of 2 atm, the reaction rate is slower, and the ignition process depends more strongly on mechanistic details, which makes the errors introduced by reduction more likely to be amplified [36]. At a pressure of 5 atm, the average relative errors of the IDT predictions obtained using Reduced Mech, Detailed Mech, and Bys-BP Mech were 20.37%, 15.98%, and 17.16%, respectively.

As shown in Figure 9b, with increasing CH_4 fraction in the fuel, the average relative error of LBV predicted by Detailed Mech decreased from 13.36% to 7.22%. The average relative error of LBV predicted by Bys-BP Mech decreased from 13.05% to 6.52%. At this stage, the combustion process is dominated by the hydrocarbon chemistry of CH_4 , while the concentration of nitrogen-containing radicals decreases and their influence on flame propagation weakens, thereby improving the prediction accuracy [37]. Error analysis

indicated that the optimized Bys-BP Mech exhibited slightly better predictive accuracy than Detailed Mech.

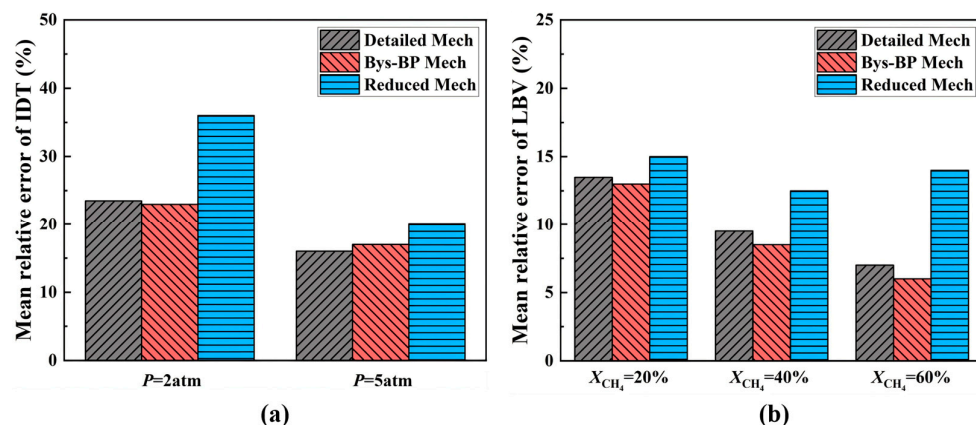


Figure 9. Mean relative errors of (a) IDT predictions under different pressures and (b) LBV predictions under different CH_4 co-firing ratios.

3.2. Performance of the Premixed Swirling Flame Based on CFD

For the NO emission characteristics of NH_3/CH_4 combustion, the predictions obtained using the Bys-BP Mech developed in this study were compared with the experimental data of Tu et al. [22] and the Modified Okafor mechanism adopted by them, as shown in Figure 10. The results showed that the prediction errors of NO emissions obtained using Bys-BP Mech were 4.84%, 3.74%, 4.64%, and 8.19% relative to the experimental measurements when the CH_4 co-firing ratio was $X_{\text{CH}_4} = 40 \sim 70\%$, respectively. Compared with the Modified Okafor mechanism, Bys-BP Mech exhibited better agreement, indicating that the optimized Bys-BP Mech could more accurately capture the effect of NH_3 co-firing on NO emissions.

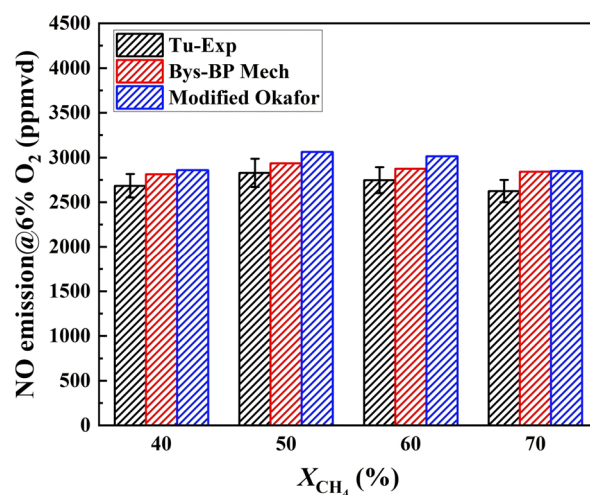


Figure 10. NO emissions under different CH_4 co-firing ratios.

In addition, gas turbines serve as critical units during peak-shaving operation, and their operating loads vary frequently, which imposes more stringent requirements on combustion stability and emission performance. Therefore, the temperature distribution inside the combustor was analyzed at heat loads of 50~100% in this study, as shown in Figure 11. As the heat load decreased, the temperature regions ranging from 1650 K to 1900 K in the combustor were noticeably reduced. This was because the inlet velocity of the combustor decreased from 2.160 m/s to 1.079 m/s, which reduced the total amount

of fuel supplied to the combustor per unit time and consequently decreased the total heat released by combustion.

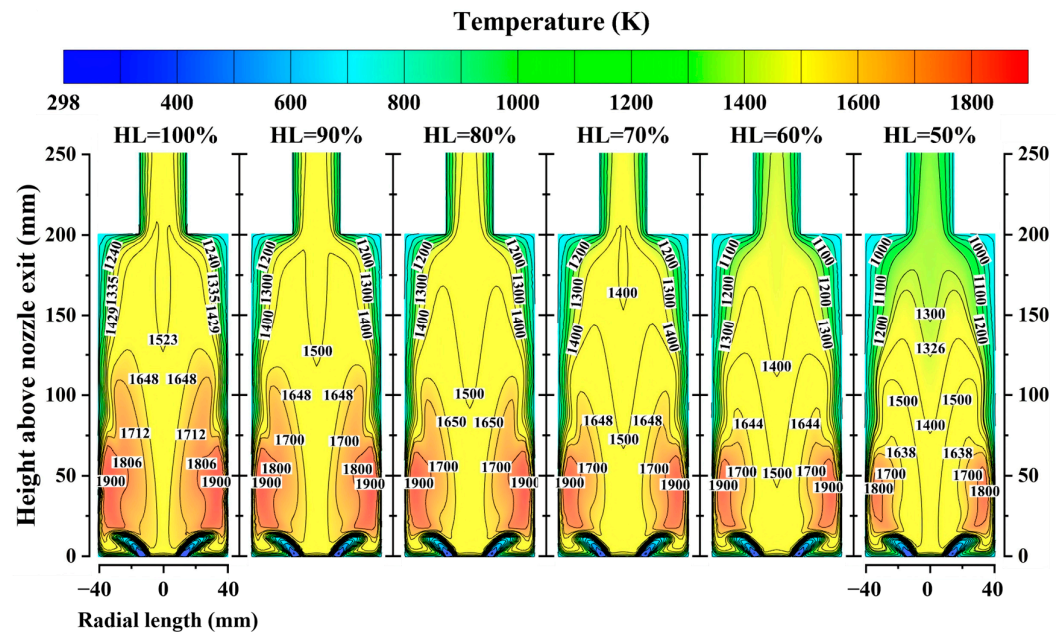


Figure 11. Temperature distribution inside the combustor under different heat loads.

Figure 12 shows the turbulent intensity under different heat loads and at different heights from the burner nozzle outlet. When the heat load was 100%, the turbulent intensity at $H = 50$ mm from the nozzle outlet reached 37.73%, which enabled the formation of a large-scale and stable high-intensity reaction zone. As the height increased, the turbulent intensity in the combustor decreased from 37.73% to 23.67%. When the heat load was 50%, the kinetic energy of the fuel jet weakened, and the turbulent intensity at $H = 50$ mm from the nozzle outlet gradually decreased to 19.92%. This reduced the spatial extent of the region capable of sustaining intense chemical reactions, and the reaction zone was more readily diluted and cooled by the surrounding airflow. Consequently, the high-temperature core region contracted [38].

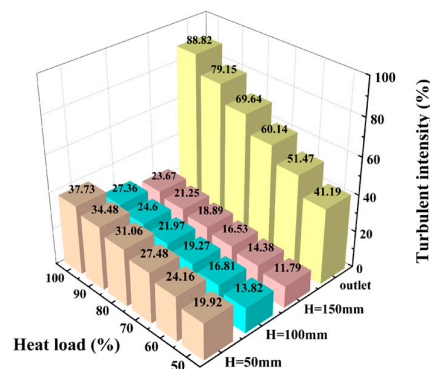


Figure 12. Turbulent intensity under different heat loads and at different heights from the nozzle outlet.

Figure 13 shows the axial flow-field distribution inside the combustor under different heat loads. When the heat load decreased from 100% to 50%, the peak velocity of the flow field inside the combustor decreased from 10.0 m/s to 4.0 m/s, and the recirculation intensity was also markedly weakened. At high heat loads, the coexistence of positive and negative velocity regions formed a steep shear layer. A strong central recirculation zone with a velocity of -2 m/s existed, as indicated by the red box in Figure 13, which ensured

hot-gas recirculation and mixing efficiency and was conducive to flame stabilization. As the load decreased, the strong central recirculation region gradually contracted, and its velocity decreased to -1 m/s, resulting in a corresponding reduction in the recirculation-zone area.

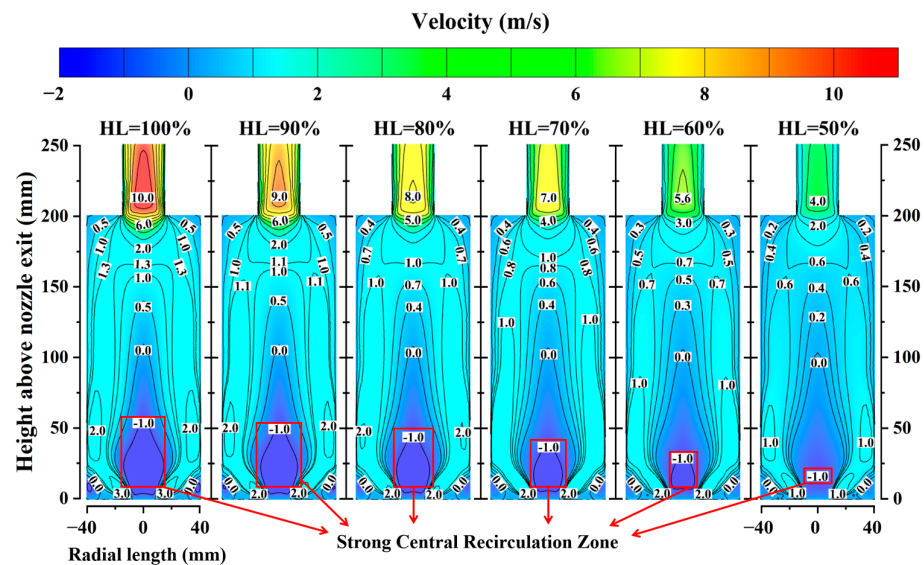


Figure 13. Axial flow-field distribution inside the combustor under different heat loads.

Figure 14 shows the area fraction of the recirculation zone under different heat loads. As the heat load decreased, the area fractions of the recirculation zone were 16.05%, 16.04%, 15.81%, 15.63%, 15.54%, and 15.37%, respectively, showing a downward trend. When the heat load decreased to 50%, the inlet mass flow rate and momentum decreased most significantly, while the diffusion effect was relatively enhanced. As a result, the velocity exhibited a more uniform spatial distribution. This was coupled with the contraction and homogenization of the reaction zone in the temperature field, jointly explaining the evolution of combustion characteristics under variable-load conditions.

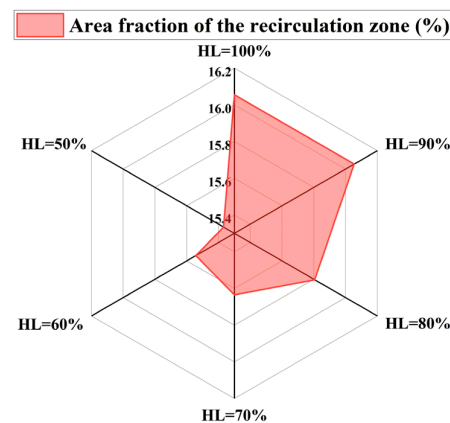


Figure 14. The area fraction of the recirculation zone under different heat loads.

Figure 15 shows the variation in NO emissions under different heat loads and at different heights from the nozzle outlet. Overall, NO emissions decreased as the heat load decreased, because the formation rate of thermal NO exhibits an exponential dependence on temperature [18]. Therefore, the reduction in combustion temperature directly suppressed the thermal NO formation pathway. Meanwhile, the decrease in heat load significantly weakened the central recirculation intensity, and the area fraction of the recirculation zone decreased from 16.05% to 15.37%, which reduced the entrainment and

preheating effects of high-temperature products on the flame root. In addition, the attenuation of turbulent intensity shifted the combustion mode toward diffusion-controlled dominance and prolonged the reaction process, thereby suppressing NO formation from the kinetic perspective.

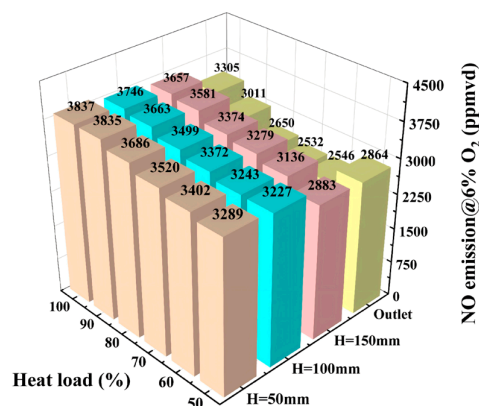


Figure 15. NO emissions under different heat loads and at different heights from the nozzle outlet.

It is noteworthy that NO emissions at the outlet section exhibited an abnormal rebound at 50% load, increasing from 2546 ppmvd to 2864 ppmvd, which was approximately 12.49% higher than that at 60% load. This phenomenon was mainly attributed to the weakened central recirculation zone and reduced turbulence intensity under low-load conditions, which formed a flow-field environment characterized by an overall low temperature, locally nonuniform mixing, and a prolonged reaction process. On the one hand, this prolonged the residence time of NO in the downstream region. On the other hand, it made low-temperature conditions more favorable for the competition of the N_2O -mediated pathway, thereby promoting the continuous formation of NO downstream [39]. In addition, under low-load conditions, the thermal transport and diffusion effects of the gas flow were relatively enhanced, local heat loss was reduced, and fuel–oxidizer mixing efficiency was improved, which also promoted NO formation under this operating condition to some extent. Verification showed that the mole fractions of CH_4 and NH_3 at the combustor outlet were below the order of 10^{-6} over the entire heat-load variation range, indicating that the fuels had been completely consumed inside the combustor.

4. Conclusions

This study combined ANN with Bayesian optimization and proposed a data-driven parameter optimization method for the NH_3/CH_4 combustion reaction mechanism. A new optimized mechanism, Bys-BP-Mech, was constructed, and its prediction accuracy for LBV and IDT was validated, which improved the generalization capability of the mechanism across a wide range of pressure conditions. Meanwhile, the optimized mechanism was applied to CFD simulations to analyze the combustion characteristics and NO_x emission characteristics of NH_3/CH_4 under different heat loads, thereby addressing the deficiency of existing mechanisms in combustor-scale validation under variable operating conditions. The main conclusions are as follows:

- (1) Through sensitivity analysis of IDT, reactions R23, R57, and R79 were found to have the highest sensitivity coefficients, reaching 0.400, 0.358, and 0.280, respectively, and exhibited significant inhibiting effects.
- (2) The mean relative error of the LBV predictions obtained using Bys-BP Mech decreased from 13.05% to 6.52% as the CH_4 fraction increased when $X_{CH_4} = 20 \sim 60\%$.

- (3) The prediction errors of NO emissions obtained using Bys-BP Mech first decreased and then increased, with values of 4.84%, 3.74%, 4.64%, and 8.19%, respectively, when $X_{CH_4} = 40 \sim 70\%$.
- (4) NO emissions at the combustor outlet decreased monotonically as the heat load decreased. However, at 50% heat load, NO emissions increased from 2546 ppmvd to 2864 ppmvd, which was approximately 12.49% higher than that at 60% load. The velocity peak in the strong central recirculation zone decreased from -2 m/s to -1 m/s, and the area fraction of the recirculation zone contracted from 16.05% to 15.37%.

Current research has mainly focused on the fundamental characteristics of premixed flames and swirling combustion simulations under different heat loads. Systematic validation involving non-premixed combustion, high-pressure real gas turbine operating conditions, and a wider blending-ratio range has not yet been addressed. Future research can expand the experimental and simulation databases in these directions and introduce multiple machine learning methods to establish surrogate models for predicting combustion characteristics under wide operating conditions and multiple objectives, with the aim of improving the applicability of the mechanism.

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