

Article

Effects of Equivalence Ratio and Inlet Temperature on Combustion and NO_x Emissions of Partially Cracked Ammonia in a Cavity Micro-Combustor

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Abstract

This work numerically examines the premixed combustion of partially cracked ammonia/air in a cavity-stabilized micro-combustor. Effects of the equivalence ratio (Φ) and inlet temperature (T_{in}) on the combustion features, flame–wall heat transfer and nitrogen-containing emissions are investigated quantitatively at a cracking ratio of 0.6. Results show that increasing Φ from 0.8 to 1.2 shifts the high-temperature region downstream and causes it to elongate axially. This spatial expansion decreases peak temperatures and distributes heat release over a longer distance. Mean wall temperature and overall heat loss are thus decreased due to weakened near-wall thermal interaction. NO formation closely follows the high-temperature and OH-rich zones. However, at $\Phi = 1.2$, oxygen limitation suppresses NO production and redirects fuel-bound nitrogen towards N₂O, enhancing its outlet emissions. As T_{in} increases from 300 K to 500 K, the improved reactivity of the mixture promotes an upstream shift of the main reaction zone. The reaction zone becomes more concentrated within the cavity. Such structural changes intensify NO formation but simultaneously compress the high-temperature zone, which reduces the wall-averaged temperature and overall heat loss. In the extended downstream post-flame region, lower temperatures and limited radical activity suppress NO₂ formation and N₂O decomposition. As a result, NO₂ emissions decrease monotonically, while N₂O emissions exhibit a gradual increase. These findings provide useful insights into the effects of operating parameters on combustion stability, heat transfer and nitrogenous pollutant evolution in microscale partially cracked ammonia flames.

Keywords: partially cracked ammonia; micro-combustor; equivalence ratio; inlet temperature; pollutant emissions



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1. Introduction

Extreme weather events associated with global warming are occurring more frequently. Carbon dioxide (CO₂) emissions from combustion are considered a primary driver of this phenomenon. Consequently, reducing carbon emissions during combustion has become a critical priority for achieving carbon neutrality [1]. Chemical energy storage using hydrogen and ammonia produced from renewable sources is an effective pathway for low-carbon energy utilization. These approaches demonstrate significant potential due to their high conversion efficiency and compatibility with existing storage and transportation infrastructure [2]. Hydrogen is regarded as an ideal zero-carbon fuel because its combustion produces only water. However, its storage and transportation present significant safety

and economic challenges due to its low density, low boiling point, and high liquefaction pressure [3]. Ammonia has thus emerged as a promising hydrogen carrier due to its high energy density and ease of liquefaction [4,5]. Since ammonia combustion does not directly generate CO₂, it is also a potential fuel for zero-carbon combustion. Its application in industrial boilers, gas turbines, internal combustion engines, and fuel cells has attracted considerable attention [6,7]. Yet, burning ammonia is technically challenging due to its high ignition energy, poor flame stability and high NO_x emissions [8]. These issues limit the direct use of ammonia in traditional devices.

To address the inherent challenges associated with ammonia combustion, recent studies have extensively explored the combustion characteristics of ammonia and ammonia-blended fuels. A wide range of fundamental parameters, including ignition delay times, laminar flame speeds, and product distributions, have been systematically measured, and several detailed chemical kinetic mechanisms have been developed and validated, which provide a solid foundation for understanding ammonia combustion chemistry [9,10]. Given the intrinsically low reactivity of ammonia, hydrogen addition and partial fuel cracking have been widely recognized as effective strategies to enhance ignition and flame stability [11]. Wiseman et al. [12] demonstrated that partially cracking ammonia into an NH₃/H₂/N₂ mixture prior to combustion significantly improves ignition and overall combustion performance. Such NH₃/H₂/N₂-air flames also exhibit enhanced resistance to extinction and blow-off, particularly under turbulent conditions. Cui et al. [13] numerically investigated the effects of intake swirl in NH₃-H₂-fueled engines and reported that hydrogen enrichment markedly improves ignition reliability and combustion stability under lean conditions. By optimizing injection and ignition strategies, an indicated thermal efficiency of approximately 46% was achieved while maintaining acceptable emission levels. It should be noted that although these approaches effectively improve the flammability and stability of ammonia-based fuels, they also introduce new challenges in pollutant control. Enhancing fuel reactivity often leads to elevated flame temperatures and intensified nitrogen chemistry, thereby increasing the propensity for NO_x formation. To mitigate this issue, Zha et al. [14] proposed a mild-combustion strategy based on flow recirculation and reburning, which suppresses NO_x emissions by reducing local oxygen concentration and flame temperature, while maintaining stable combustion. Despite the substantial progress made in understanding the ignition, propagation and emission characteristics of NH₃-H₂ premixed flames, a systematic understanding of the coupled relationship between flame stabilization mechanisms and nitrogenous pollutant formation remains limited. In particular, how key control parameters simultaneously govern combustion stability and pollutant evolution has not yet been fully elucidated, motivating further investigation.

Driven by the growing demand for miniaturized and portable energy conversion devices, micro-combustors have emerged as promising platforms for utilizing ammonia-based fuels [15]. Compared with conventional power sources, micro-combustors offer high energy density, rapid thermal response, and favorable energy conversion efficiency, making them attractive heat sources for micro-thermophotovoltaic and micro-thermoelectric systems [16]. However, when the combustion scale is reduced to the millimeter level, strong non-adiabatic effects become unavoidable. Intense wall heat transfer, coupled with extremely short gas residence times, fundamentally alters flame stability, heat-release characteristics and emission behavior. As a result, combustion laws and stabilization mechanisms established at the macroscopic scale are no longer directly applicable to micro-scale systems [17]. The significantly increased surface-to-volume ratio in micro-combustors leads to severe wall heat losses and enhances flame-wall interactions, making flames more prone to extinction and reducing overall combustion efficiency [18].

To mitigate these challenges, extensive efforts have been devoted to the development of advanced combustor structures and stabilization strategies. Proper structural design can increase wall temperature, enhance heat recirculation, extend gas residence time and promote more complete fuel conversion, thereby improving thermal efficiency and flame stability. For example, Ni et al. [19] demonstrated that the introduction of internal fins or expansion channels increases the average wall temperature and reduces temperature non-uniformity, enabling flame anchoring at specific locations and improving heat transfer performance. Yan et al. [20] numerically proposed a heat-recirculating micro-combustor incorporating porous media, showing that enhanced radial heat transfer significantly elevates baffle temperature and strengthens reactant preheating. Consequently, the high-temperature reaction zone becomes more concentrated, the temperature field more uniform and the stable operating velocity range substantially extended. Despite these advances, direct micro-scale combustion of ammonia remains relatively underexplored. This is primarily due to the intrinsically low reactivity of ammonia–air mixtures, their high ignition temperature and strong extinction tendency. Moreover, stringent NO_x emission constraints often come at the expense of combustion efficiency, which conflicts with the high-efficiency requirements of micro-combustors [21,22]. Therefore, micro-scale ammonia combustion presents a coupled challenge involving flame stability, thermal efficiency, and nitrogenous pollutant control, rather than a single-parameter optimization problem.

It is also noteworthy that many existing studies treat partially cracked ammonia as equivalent to direct hydrogen blending. However, the presence of N₂ introduced during ammonia cracking, and its influence on heat transfer, flow dilution and reaction-zone structure, cannot be neglected. Beyond structural enhancement and partial cracking strategies, operating parameters also play decisive roles in determining micro-combustion performance. For partially cracked NH₃ premixed flames, the equivalence ratio directly regulates local fuel oxidation and radical pools, thereby controlling the location of the main reaction zone, heat-release intensity and the competitive formation pathways of NO, N₂O and NO₂. Meanwhile, the inlet temperature affects the flow reactivity and the demand for heat recirculation, influencing flame establishment, wall thermal response and downstream temperature decay. To address these interactions, the present study numerically investigates the coupled effects of equivalence ratio (Φ) and inlet temperature (T_{in}) on the combustion characteristics, flame stability and nitrogenous pollutant evolution in partially cracked NH₃/air premixed combustion at the micro-scale. The results are expected to provide fundamental insights into micro-scale ammonia combustion and offer practical guidance for the design of micro-combustors with low emissions, high efficiency and enhanced flame stability.

2. Numerical Methods

2.1. Numerical Model and Computational Setup

Figure 1 illustrates the geometric configuration of the micro-combustor. The device consists of a straight inlet section followed by a downstream channel, with a recessed cavity embedded between them. The cavity is designed to induce a stable recirculation zone, which serves as an effective flame anchoring location and enhances flame stability under the strong heat-loss conditions inherent to micro-scale combustion. The key geometric parameters are defined in the figure. The total length of the combustor (L_1) is 18 mm. The inlet height (D_1) is 1 mm, and the wall thickness (D_3) is 2 mm. The distance from the inlet to the upstream edge of the cavity (L_2) is 3 mm. The cavity has a length (L_3) of 3 mm, a depth (D_2) of 1 mm, and a ramp angle (θ) of 45°.

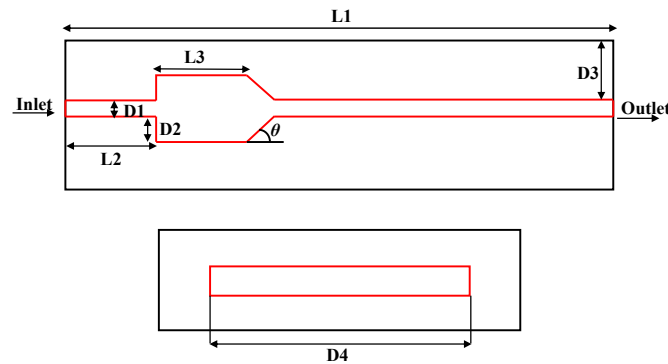


Figure 1. Geometric schematic of the micro-combustor.

Given the significant heat losses inherent to micro-combustors [23], conjugate heat transfer is included by solving wall conduction and accounting for heat exchange between the inner and outer wall surfaces. Quartz glass is selected as the wall material, and its thermophysical properties are specified as follows: a specific heat (C_p) of 750 J/(kg·K), a density (ρ) of 2650 kg/m³, and a thermal conductivity (k_s) of 1.05 W/(m·K) [24]. The inlet mixture consists of partially cracked ammonia and air, which are treated as ideal gas. In this study, partially cracked ammonia is quantified by the ammonia cracking ratio (α), which represents the fraction of initial NH₃ decomposed into H₂ and N₂. In practical NH₃ cracking systems, achieving complete conversion is energy-intensive and challenging; therefore, the combustor inlet is commonly a mixed NH₃/H₂/N₂ stream rather than a fully cracked gas. Accordingly, a fixed cracking ratio of $\alpha = 0.6$ is selected as a representative operating condition, meaning that 60% of the ammonia is cracked while 40% remains. This corresponds to a specific inlet fuel composition with a hydrogen-to-ammonia molar ratio of H₂/NH₃ = 9:4, and the N₂ fraction is determined by the stoichiometry of the cracking reaction. The specific heat capacity of the gas mixture is evaluated using the mixing law, while viscosity and thermal conductivity are calculated using mass-weighted averaging methods [25]. For species transport, a mixture-averaged formulation is employed, where diffusion coefficients are evaluated based on kinetic theory [26]. The operating pressure is set to 1 atm. At the inlet, a velocity-inlet boundary condition is applied with a uniform flow velocity of 4 m/s, and the inlet temperature (T_{in}) varies from 300 to 500 K, specifically 300, 350, 400, 450, and 500 K. To facilitate a clear overview of the numerical framework, the detailed boundary conditions in the simulations are summarized in Table 1. A pressure-outlet boundary condition is utilized at the combustor exit, and no-slip conditions are enforced at all gas–solid interfaces. The discrete ordinates (DO) radiation model is employed to calculate the radiative heat exchange between the participating media and the internal walls [27]. Heat exchange between the outer wall and the ambient environment is calculated using the following correlation [28,29]:

$$Q = h(T_w - T_\infty) + \varepsilon_{wall}\sigma(T_w^4 - T_\infty^4) \quad (1)$$

where h represents the natural-convection heat-transfer coefficient, set to 20 W/(m²·K) [30]. The wall emissivity, ε_{wall} , is set to 0.92 for quartz glass, while T_w and T_∞ denote the outer-wall temperature and ambient temperature. σ is the Stefan–Boltzmann constant (5.67×10^{-8} Wm⁻²·K⁻⁴).

The characteristic length (L_c) of the micro-combustor is significantly larger than the molecular mean free path (λ). Consequently, the calculated Knudsen number (Kn) falls within the continuum regime [31], which justifies the application of the Navier–Stokes equa-

tions in this study. Accordingly, the governing equations include continuity, momentum, energy conservation and chemical species transport, expressed as follows [32]:

Table 1. Boundary conditions for the numerical simulation.

Items	Settings
Inlet of the combustor	Uniform concentration and velocity distributions at 4 m/s, 300–500 K, 1 atm, $\alpha = 0.6$ and $\Phi = 0.8$ –1.2
Combustion chamber wall	Coupled boundary with no-slip
External wall surface of the combustor	Mixed (convection + radiation), ambient temperature of 300 K, wall emissivity of 0.92 and heat transfer coefficient of 20 W/(m ² ·K)
Outlet of the combustor	Pressure outlet
Combustor wall properties	Quartz, density of 2650 kg/m ³ , specific heat of 750 J/(kg·K) and thermal conductivity of 1.05 W/(m·K)

Continuity equation:

$$\frac{\delta \rho}{\delta t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (2)$$

Momentum conservation equation:

$$\frac{\delta}{\delta t} (\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\bar{\tau}) + \rho \vec{g} + \vec{F} \quad (3)$$

where ρ represents density, and $\bar{\tau}$ is the viscous stress tensor. The term $\rho \vec{g}$ denotes the gravitational body force per unit volume, while $\vec{F}$ is the external body force.

Energy conservation equation:

$$\frac{\delta}{\delta x_j} (\rho u_j h + F_{hj}) = u_j \frac{\delta \rho}{\delta x_j} + \tau_{ij} \frac{\delta u_i}{\delta x_j} \quad (4)$$

where h is the specific enthalpy of the gas mixture, F_{hj} indicates the energy flux in the x_j direction, and τ_{ij} and u_i correspond to the stress tensor and the velocity component, respectively.

Species transport equation:

$$\frac{\delta}{\delta t} (\rho Y_i) + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot \vec{J}_i + R_i \quad (5)$$

where Y_i , R_i and $\vec{J}_i$ denote the mass fraction, consumption rate, and diffusive flux of species i , respectively.

Because heat conduction within the combustor wall has a significant influence on flame stability in micro-scale systems [33], heat conduction in the solid domain is explicitly accounted for in the present simulation model. The corresponding solid-phase energy equation is expressed as follows [34]:

$$\frac{\partial (\rho_s c_s T_s)}{\partial t} = \frac{\partial (k_s \partial T_s)}{\partial x^2} + \frac{\partial (k_s \partial T_s)}{\partial y^2} \quad (6)$$

where k_s denotes the thermal conductivity of the solid, C_s denotes the specific heat capacity, and T_s denotes the temperature.

In this study, ANSYS Fluent 15.0 is employed to simulate fluid flow, combustion and heat transfer within the micro-combustor. The governing equations are solved using the finite-volume method. The realizable k - ϵ turbulence model is selected for this study, as previous investigations have demonstrated its superior capability in capturing turbulent flow dynamics within micro-combustors [35,36]. All results reported in this study were obtained from steady-state simulations. Gradients are evaluated with a least-squares cell-based scheme, while pressure interpolation employs a second-order scheme. The convective terms in the momentum, energy, species, and turbulence equations are discretized using second-order upwind schemes. Pressure–velocity coupling is handled using the SIMPLE algorithm, and the chemical source terms are treated using a stiff chemistry solver. Combustion chemistry is described using the Stagni reaction mechanism [37], which includes 31 species and 161 elementary reactions for NH_3/H_2 mixtures. This mechanism has been widely validated and has demonstrated good predictive capability for NH_3/H_2 combustion processes. To facilitate the analysis of pollutant formation mechanisms in the subsequent sections, the principal elementary reactions governing NH_3 oxidation, NO formation, and N_2O production are extracted from the full mechanism and listed in Table 2. The convergence criterion for all residuals is uniformly set to 10^{-6} .

Table 2. Representative elementary reactions for NH_3 oxidation and NO_x speciation.

Group	ID	Elementary Reaction
NH_3 consumption/ NH_i formation	R1	$\text{NH}_3 + \text{H} = \text{NH}_2 + \text{H}_2$
	R2	$\text{NH}_3 + \text{OH} = \text{NH}_2 + \text{H}_2\text{O}$
	R3	$\text{NH}_3 + \text{O} = \text{NH}_2 + \text{OH}$
	R4	$\text{NH}_2 + \text{OH} = \text{NH} + \text{H}_2\text{O}$
NO formation	R5	$\text{NH} + \text{O} = \text{NO} + \text{H}$
	R6	$\text{N} + \text{OH} = \text{NO} + \text{H}$
	R7	$\text{N} + \text{O}_2 = \text{NO} + \text{O}$
	R8	$\text{NH} + \text{OH} = \text{HNO} + \text{H}$
	R9	$\text{NH} + \text{O}_2 = \text{HNO} + \text{O}$
	R10	$\text{NH}_2 + \text{O} = \text{HNO} + \text{H}$
	R11	$\text{NH}_2 + \text{O}_2 = \text{HNO} + \text{OH}$
	R12	$\text{HNO} + \text{H} = \text{NO} + \text{H}_2$
	R13	$\text{HNO} + \text{O} = \text{NO} + \text{OH}$
	R14	$\text{HNO} + \text{OH} = \text{NO} + \text{H}_2\text{O}$
NO_2 formation	R15	$\text{NO} + \text{HO}_2 = \text{NO}_2 + \text{OH}$
	R16	$\text{NO} + \text{O} (+\text{M}) = \text{NO}_2 (+\text{M})$
	R17	$\text{NO}_2 + \text{H} = \text{NO} + \text{OH}$
N_2O formation	R18	$\text{NH} + \text{NO} = \text{N}_2\text{O} + \text{H}$
	R19	$\text{NH}_2 + \text{NO}_2 = \text{N}_2\text{O} + \text{H}_2\text{O}$

To systematically investigate the effects of operating parameters on combustion stability and emissions, the present study focuses on two key variables while keeping the combustor geometry and other boundary conditions unchanged, namely the equivalence ratio (Φ) and the inlet temperature (T_{in}). It is noted that flame stability in this work is assessed in terms of whether the flame remains stably anchored in the intended stabilization region under the investigated operating conditions. The equivalence ratio, which characterizes the fuel–air mixture strength, is varied by fixing the ammonia cracking ratio at 0.6 and selecting three representative values, $\Phi = 0.8, 1.0$, and 1.2 , to evaluate their influences on flame stability and nitrogenous pollutant formation. Meanwhile, the inlet temperature, a critical parameter governing ignition propensity and chemical reaction rates, is varied from 300 to 500 K (300, 350, 400, 450, and 500 K) under the same cracking ratio.

2.2. Mesh Independence and Model Validation

A mesh-sensitivity study was performed to ensure that the numerical predictions are independent of grid resolution. Four computational meshes were generated with minimum grid sizes of 25 μm , 20 μm , 15 μm , and 10 μm , corresponding to total cell counts of approximately 23,000, 51,231, 70,490, and 112,090, respectively. As shown in Figure 2, the coarsest mesh (23,000 cells) produces noticeable deviations in the centerline temperature distribution. With grid refinement, the temperature profiles gradually converge. In particular, the results obtained using meshes with 51,231 cells or more are nearly indistinguishable, indicating grid-independent solutions. Therefore, to achieve a balance between computational accuracy and efficiency, the mesh containing 70,490 cells was selected for all subsequent simulations.

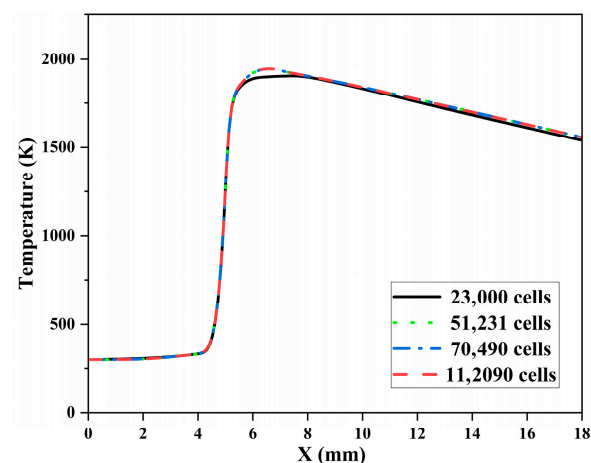


Figure 2. Comparison of centerline temperature profiles obtained with four mesh resolutions (23,000, 51,231, 70,490, and 112,090 cells).

The numerical model was validated against experimental data reported in Ref. [38], as shown in Figure 3. Specifically, the predicted outlet temperatures of an H_2/air flame at an equivalence ratio of $\Phi = 0.3$ were compared with experimental data over a range of inlet velocities from 8 to 24 m/s. Since no experimental error bars were shown in the original dataset, representative uncertainty bands ($\pm 5\%$) were added to facilitate a clearer comparison between the experimental and numerical results. The numerical results exhibit good agreement with the experimental data, capturing the overall trends accurately. The deviations in outlet temperature remain within 5% across the entire velocity range, demonstrating the reliability of the present model for the subsequent parametric investigation.

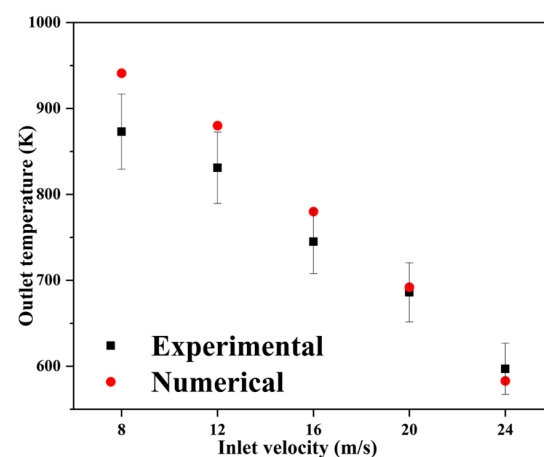


Figure 3. Comparison of simulated and measured outlet temperatures at various inlet velocities.

3. Results and Discussion

3.1. Effects of the Equivalence Ratio

Figure 4 illustrates pronounced differences in the location and morphology of the high-temperature region under different equivalence ratios. At $\Phi = 0.8$ and $\Phi = 1.0$, a well-defined high-temperature core is established within the cavity, indicating that the cavity effectively anchors the primary reaction zone under these conditions. Although the overall thermal intensity is comparable in the two cases, slight variations are observed in the shape and axial extent of the high-temperature region. When the equivalence ratio is increased to $\Phi = 1.2$, the high-temperature region moves downstream in the axial direction, accompanied by a reduction in the peak temperature. This behavior suggests that under fuel-rich conditions, oxygen deficiency leads to a more distributed heat-release process, thereby reducing the local reaction rate and extending the burnout process further downstream. Overall, increasing Φ results in a downstream shift of the primary high-temperature region. Sun et al. [39] also demonstrated that the equivalence ratio significantly influences the temperature field in a CH_4/NH_3 -fueled micro-planar combustor. In their study, the variation is primarily manifested as changes in thermal intensity, with the high-temperature region remaining near the upstream side and becoming stronger under near-stoichiometric conditions. In contrast, the present cavity combustor exhibits a more pronounced downstream shift and spatial redistribution of the primary high-temperature region under fuel-rich conditions. This distinction arises from the different flame-stabilization mechanisms. In the present configuration, the primary reaction zone is stabilized by cavity-induced recirculation. When Φ increases to fuel-rich conditions, oxygen deficiency weakens the local heat release and promotes a more distributed oxidation process, thereby delaying fuel burnout and shifting the high-temperature region downstream. By comparison, in the micro-planar combustor studied by Sun et al., the temperature-field response is predominantly governed by planar flame stabilization near the inlet, where variations in equivalence ratio mainly modulate thermal intensity rather than the axial position of the reaction zone.

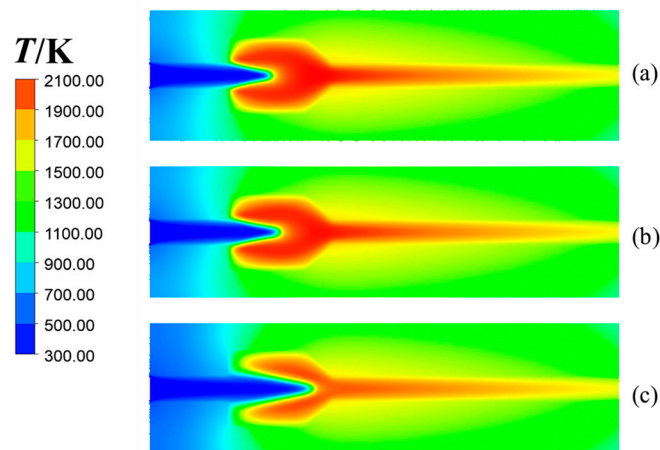


Figure 4. Temperature contour distributions at different Φ : (a) $\Phi = 0.8$, (b) $\Phi = 1.0$, (c) $\Phi = 1.2$.

To quantitatively analyze the axial shift of the reaction zone observed in Figure 4, Figure 5a presents the centerline temperature distributions under different equivalence ratios, while Figure 5b illustrates the corresponding centerline heat release rate profiles. As Φ increases from 0.8 to 1.2, both the onset of the rapid temperature rise and the location of the peak temperature progressively move downstream, providing quantitative confirmation of the downstream migration of the primary reaction zone. In terms of peak temperature, the highest value is obtained at $\Phi = 0.8$, with the peak at $\Phi = 1.0$ being only slightly lower. This is because, at moderately lean conditions, sufficient oxygen availability combined with

sufficient thermal feedback in the cavity promotes more complete and intense oxidation reactions, leading to higher localized heat release. As shown in Figure 5b, for $\Phi = 0.8$, the primary reaction zone is anchored further upstream within the cavity, and the peak centerline heat-release rate is higher than that for $\Phi = 1.0$. This more upstream and localized heat release results in a more substantial temperature rise within the cavity, consistent with the higher peak centerline temperature observed in Figure 5a. In contrast, a pronounced reduction in peak temperature is observed at $\Phi = 1.2$. This discrepancy indicates that, for $\Phi = 0.8$ – 1.0 , heat release remains strong and spatially concentrated within the cavity, resulting in a sharp temperature rise over a short axial distance. Under fuel-rich conditions, oxygen deficiency leads to a more distributed heat-release process and delayed burnout, as reflected by the lower peak temperature and the extended axial temperature profile.

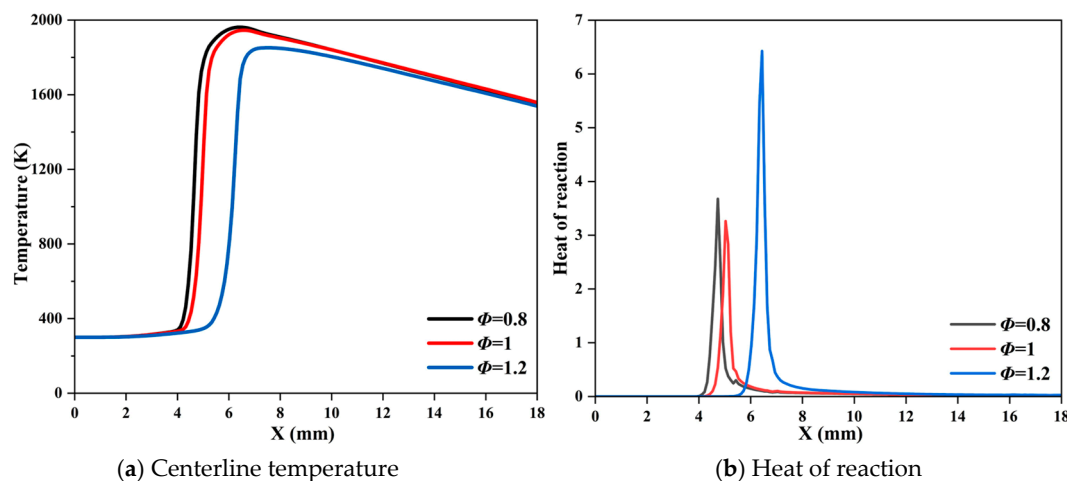


Figure 5. Axial distribution of the combustor centerline temperature and centerline heat of reaction at different Φ .

OH radicals are selected as the primary reaction-zone indicator in this study, as they are widely recognized as reliable markers of the high-temperature reaction zone and are closely correlated with the volumetric heat-release region in premixed combustion [40]. As shown in Figure 6, regions of elevated OH concentration closely coincide with areas of steep temperature gradients, further confirming the axial shift of the primary reaction zone identified in Figures 4 and 5. At $\Phi = 0.8$, a distinct high-OH region is established within the cavity. This can be attributed to the combined effects of sufficient oxygen availability for OH formation, which sustains the strong chemical reactivity in the cavity. When Φ increases to 1.0, the high-OH region remains anchored within the cavity but becomes more spatially compact with sharper boundaries. This reflects an optimal balance between fuel availability, oxygen concentration and thermal feedback, leading to intensified but more localized radical production. In addition, at $\Phi = 1.2$, the overall OH concentration is significantly reduced, and the high-OH region shifts further downstream from the cavity. This reduction is attributed not only to the downstream migration of the reaction zone but also to the intrinsic suppression of OH formation under fuel-rich conditions, where oxygen deficiency limits chain-branching reactions involving O and OH radicals. Consequently, the reaction zone weakens and becomes more spatially distributed, extending downstream in the axial direction. To further verify this reaction zone behavior, the volumetric heat-release rate distributions are evaluated and presented in Figure 7. These results directly confirm both the migration and the compression of the reaction zone. Specifically, as the equivalence ratio increases, the region of peak volumetric heat release shifts downstream,

exhibiting a spatial evolution that is fully consistent with the high-temperature and OH-radical distributions.

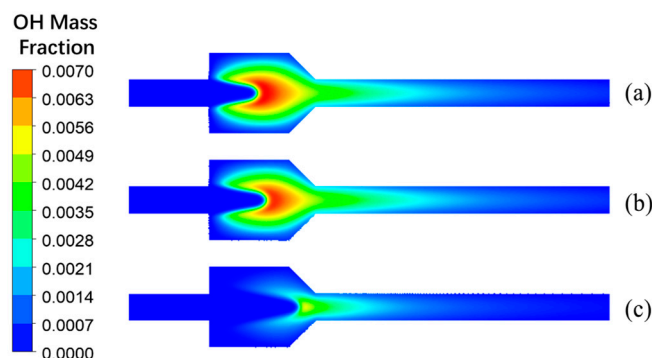


Figure 6. OH radical distributions at different Φ : (a) $\Phi = 0.8$, (b) $\Phi = 1.0$, (c) $\Phi = 1.2$.

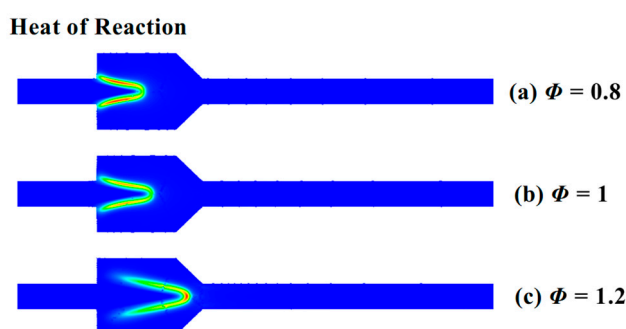


Figure 7. Heat of reaction at different Φ : (a) $\Phi = 0.8$, (b) $\Phi = 1.0$, (c) $\Phi = 1.2$.

Changes in the equivalence ratio not only directly affect combustion processes by altering chemical kinetics, but also indirectly influence them by modifying flame–wall thermal coupling. As shown in Figure 8, the average wall temperature and heat loss exhibit similar levels for $\Phi = 0.8$ and $\Phi = 1.0$, with only minor differences. Under these conditions, relatively strong chemical reactivity is sustained within the cavity, allowing the recirculation zone to effectively anchor a compact high-temperature reaction region. The resulting intense gas-phase heat release maintains a large temperature gradient between the flame and the wall, leading to comparable wall heating and external heat loss.

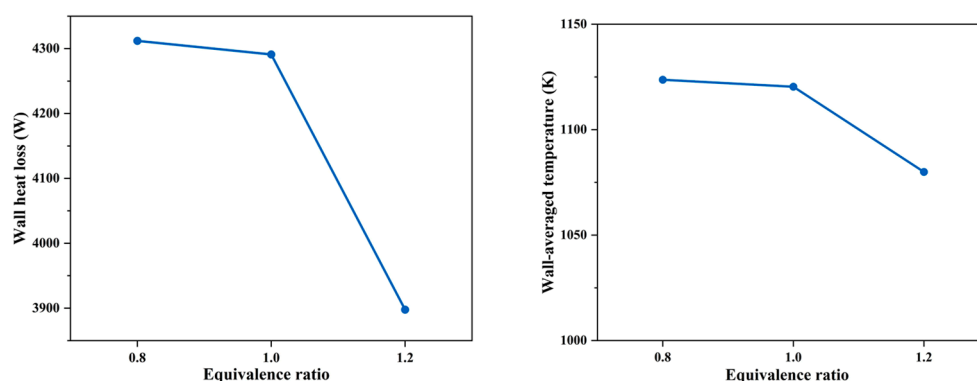


Figure 8. Wall heat loss and wall-averaged temperature at different Φ .

When the equivalence ratio is increased to $\Phi = 1.2$, both the average wall temperature and heat loss decrease markedly. From a chemical perspective, insufficient oxygen in fuel-rich conditions can suppress reaction rates and active radical production to some extent, which weakens the local heat release intensity. Moreover, the primary reaction zone

shifts downstream from the cavity into the narrow straight channel, where the absence of cavity-induced recirculation and the reduced combustion intensity jointly limit the effective residence time and thermal feedback. Here, the residence time represents the characteristic flow timescale derived from the local axial velocity. It is noteworthy that although the inlet velocity is fixed, the variations in heat release and gas density at different equivalence ratios modify the local flow acceleration, thereby altering the effective residence time experienced by the reacting mixture. As a result, heat release becomes weaker and more distributed, leading to smaller temperature gradients. Heat transfer between the wall and the flow is thus reduced, contributing to lower wall temperatures and decreased heat loss. This rich-side weakening of the wall thermal response is partly consistent with the trend reported by Nauman et al. [41] for a CH_4/H_2 catalytic micro-combustor, where the wall temperature reaches a maximum near stoichiometric conditions and then decreases under fuel-rich conditions. However, the present $\text{NH}_3/\text{H}_2/\text{N}_2$ -air system is also affected by fuel-nitrogen chemistry and cavity-stabilized gas-phase heat release, so the magnitude of the variation is not expected to be the same.

Variations in Φ significantly affect the formation and spatial distribution of nitrogenous pollutants in the micro-combustor. As shown in Figure 9, both the morphology and location of high-NO concentration zones vary markedly with Φ . At $\Phi = 0.8$ and $\Phi = 1.0$, regions of elevated NO concentration are mainly confined within the cavity and the downstream zone. Under these conditions, NO formation is strongly coupled with the high-temperature reaction core stabilized in the cavity, where sufficient oxygen availability and abundant O/OH radicals promote thermal- and fuel-NO formation pathways. Convective transport further distributes the generated NO into the wake region.

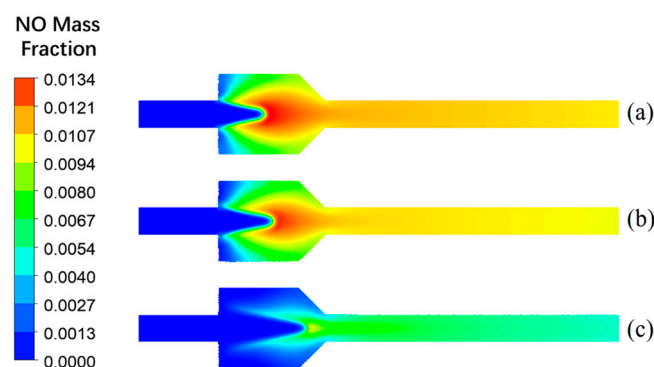


Figure 9. NO radical distributions at different Φ : (a) $\Phi = 0.8$, (b) $\Phi = 1.0$, (c) $\Phi = 1.2$.

When Φ is increased to 1.2, both the intensity and spatial extent of the high-NO zone decrease significantly, and its onset shifts further downstream. This suppression of NO formation under fuel-rich conditions can be explained as follows. First, oxygen deficiency and a relatively reduced radical pool weaken the dominant NO formation pathways. Second, the downstream displacement of the main reaction zone is accompanied by lower peak temperatures, further limiting thermal NO production. More importantly, the elevated concentration of unburned NH_3 enhances NO reduction through NO reburning reactions, which effectively consume NO in the post-flame region. The combined influence of reduced formation and enhanced consumption mechanisms results in significantly lower NO levels under fuel-rich conditions. This trend is consistent with Cai et al. [42], who also reported a marked decrease in outlet NO concentration with increasing Φ in an NH_3/O_2 micro-planar combustor.

Figure 10 presents the outlet concentrations of N_2O and NO_2 as functions of the equivalence ratio. As Φ increases from 0.8 to 1.0, the outlet N_2O concentration decreases slightly, whereas NO_2 shows a modest increase. However, at $\Phi = 1.2$, the N_2O emissions

rise notably. In particular, the NO_2 emissions exhibit extremely low levels across different equivalence ratios. These trends reflect the coupled influences of temperature level, oxidizing environment and the availability of key radicals (O , OH , and HO_2) on the kinetic competition involving the representative reactions listed in Table 2.

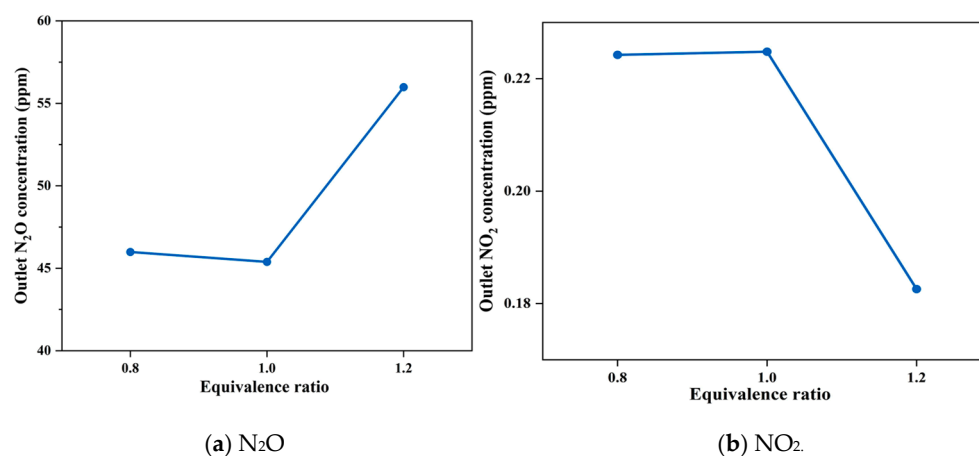


Figure 10. Outlet concentrations of N_2O and NO_2 at different Φ .

Under leaner conditions ($\Phi = 0.8$), NO formation is primarily governed by fuel-nitrogen chemistry originating from NH_3 . In the present strongly non-adiabatic micro-combustor, NO production is mainly controlled by the decomposition and oxidation pathways of nitrogen-bearing intermediates (e.g., NH , NH_2 , HNO), whose conversion to NO depends strongly on local radical availability (especially OH) and reaction-zone location. The elevated temperature levels facilitate rapid fuel-N conversion to NO while simultaneously enhancing the thermal decomposition of N_2O , thereby limiting its accumulation. By contrast, the extremely low levels of NO_2 concentrations are caused by the fact that high-temperature chemistry favors direct NO formation and suppresses the low-temperature oxidation routes required for NO -to- NO_2 conversion. Moreover, the short gas residence time and limited availability of HO_2 radicals in the wake region further restrict secondary NO oxidation, preventing noticeable NO_2 accumulation in the burned gases.

As Φ increases towards unity, the moderate reduction in peak temperature suppresses the thermal decomposition of N_2O , allowing a slightly larger fraction of N_2O to persist to the outlet. Meanwhile, the relative importance of low-temperature oxidation pathways increases. In particular, the NO formed in the main reaction zone can be further oxidized to NO_2 through reactions involving HO_2 radicals (R15: $\text{NO} + \text{HO}_2 = \text{NO}_2 + \text{OH}$), whose concentration becomes more pronounced under stoichiometric conditions. This thus contributes to a slight increase in NO_2 concentration, despite its extremely low levels.

When Φ is further increased to 1.2, oxygen deficiency, reduced flame temperature and elevated concentrations of unburned NH_3 and NH_i species jointly suppress net NO formation. In addition to weakened oxidation pathways, NO is more effectively consumed through NO reburning reactions, significantly reducing the NO pool available for subsequent oxidation. Under these fuel-rich conditions, the lower temperature and weakened oxidizing environment strongly inhibit NO_2 formation, which relies on secondary oxidation of NO through HO_2 -related pathways. As a result, NO_2 concentration at the outlet decreases markedly. In contrast, N_2O exhibits a different response. The suppression of high-temperature thermal decomposition, combined with incomplete oxidation of fuel-nitrogen intermediates under oxygen-deficient conditions, allows a larger fraction of N_2O formed via low-temperature NH_i pathways (dominated by R18: $\text{NH} + \text{NO} = \text{N}_2\text{O} + \text{H}$ and R19: $\text{NH}_2 + \text{NO}_2 = \text{N}_2\text{O} + \text{H}_2\text{O}$) to survive and be transported downstream. Furthermore, the

downstream shift of the reaction zone and the limited residence time in the post-flame region restrict the further conversion of N_2O to NO , promoting its accumulation at the outlet. Consequently, while the NO_2 concentration decreases significantly at $\Phi = 1.2$, N_2O shows a relative increase, reflecting the divergence in formation and consumption mechanisms among different NO_x species under fuel-rich conditions.

3.2. Effects of the Inlet Temperature

Figure 11 illustrates that increasing T_{in} significantly alters the location and spatial morphology of the high-temperature zone within the micro-combustor. At $T_{\text{in}} = 300$ K, the high-temperature region appears farther downstream from the cavity, indicating that the incoming mixture requires a certain axial distance for preheating and radical accumulation before entering the rapid heat release stage. As T_{in} increases to 500 K, the onset of the high-temperature zone gradually shifts upstream and develops at an earlier axial location. Elevated inlet temperature enhances chemical reactivity by accelerating fuel decomposition and chain-branching reactions, which shorten the ignition delay and promote earlier flame establishment. As a result, the main reaction zone is effectively anchored within the cavity, enabling earlier ignition and more concentrated heat release.

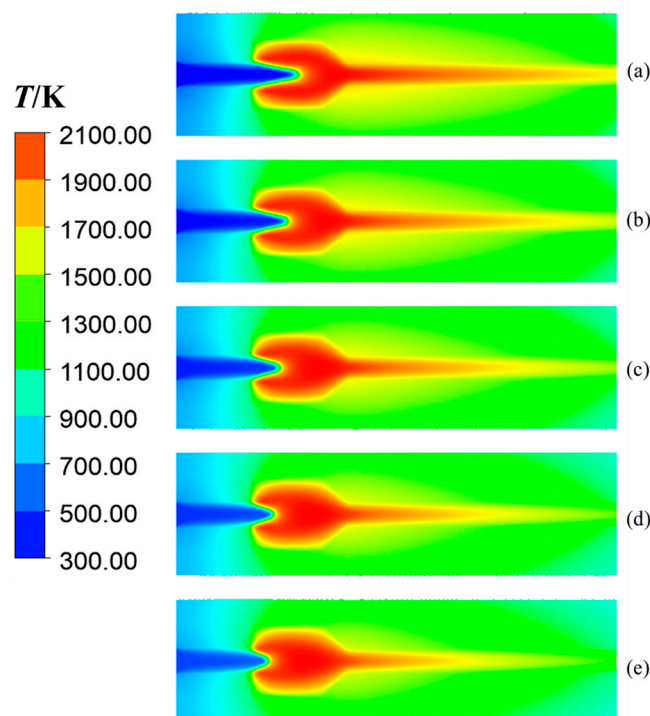


Figure 11. Temperature contour distributions at different T_{in} : (a) $T_{\text{in}} = 300$ K, (b) $T_{\text{in}} = 350$ K, (c) $T_{\text{in}} = 400$ K, (d) $T_{\text{in}} = 450$ K, (e) $T_{\text{in}} = 500$ K.

To quantify the axial shift of the main reaction zone, Figure 12 presents centerline temperature profiles for various T_{in} . As T_{in} increases, the centerline temperature enters the rapid-rise stage earlier upon reaching the cavity, and the entire steep temperature-rise segment shifts upstream. This behavior indicates that inlet preheating enables the mixture to reach the thermochemical conditions required for intense heat release more rapidly, thereby advancing the main reaction zone. This trend is consistent with the spatial temperature distributions shown in Figure 11, where the high-temperature region forms progressively earlier within the cavity.

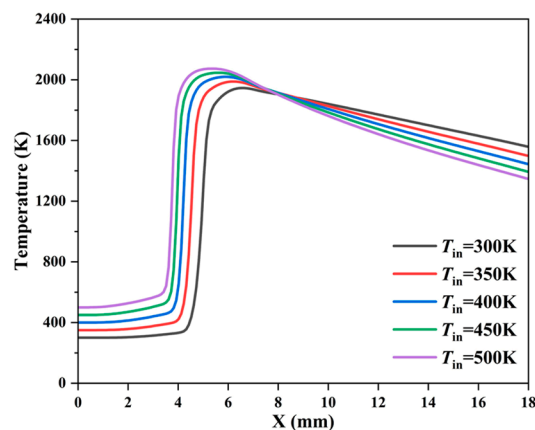


Figure 12. Axial distribution of the combustor centerline temperature at different T_{in} .

With respect to peak characteristics, the maximum centerline temperature increases gradually with T_{in} , reaching its highest value at $T_{in} = 500$ K. This reflects enhanced chemical reactivity and more intense heat release in the primary reaction zone under stronger inlet preheating. Notably, despite the increase in peak temperature, the centerline temperature decays more rapidly in the downstream channel for higher T_{in} cases, resulting in a lower outlet temperature. This somewhat unexpected trend arises because the upstream shift of the reaction zone exposes the hot combustion products to a longer downstream cooling length. Consequently, the longer residence time of the hot products enhances convective heat transfer to the walls and radiative losses, leading to a more significant temperature decay along the axial direction. It is also observed that the centerline temperature profiles for all cases tend to converge and intersect at approximately $x \approx 8$ mm. This convergence reflects a transition from a reaction-dominated regime to a cooling-controlled regime in the downstream channel. Since the primary heat release is confined within the cavity, the downstream temperature evolution is mainly governed by heat extraction to the walls. As T_{in} increases, the upstream shift of the reaction zone effectively extends the downstream cooling length, leading to a faster temperature decay along the centerline. Consequently, the temperature profiles of different T_{in} cases merge at this specific axial location due to the balance between earlier heat release and prolonged cooling.

Figure 13 illustrates the distributions of OH radicals in the micro-combustor under different T_{in} conditions. Significant differences are observed under varying T_{in} conditions. It is seen that, as T_{in} increases, the region of elevated OH radical concentration evolves from a relatively dispersed distribution to a more concentrated zone within the cavity. This indicates that higher inlet temperatures enhance chemical reactivity efficiently by accelerating fuel decomposition and chain-branching reactions, promoting earlier establishment of a highly reactive zone. Consequently, the primary combustion zone shifts upstream, resulting in a more spatially concentrated region of OH production and consumption. The resulting compact combustion zone not only strengthens local heat release but also improves flame anchoring within the cavity, highlighting the coupled effect of increased reactivity and shortened preheating distance on stabilizing micro-scale combustion.

Figure 14 shows that increasing T_{in} from 300 K to 500 K leads to a monotonic reduction in both wall heat loss and wall-averaged temperature. Although the higher inlet temperature introduces more enthalpy into the system, the reduction in net heat loss is primarily driven by the structural change of the flame. For the higher T_{in} condition, although the local peak temperature is elevated noticeably within the main reaction zone, the reaction zone also moves upstream, which leads to a more spatially concentrated high-temperature region. Under such conditions, the primary reaction zone shifts upstream and becomes axially compressed, causing the downstream channel to enter the cooling region earlier.

Although the local peak temperature increases, the wall is exposed to intense heating over a shorter length, which lowers the wall-averaged temperature. Consequently, the overall temperature difference between the outer wall and the ambient is reduced, leading to diminished convective and radiative heat losses. In contrast, Zhang et al. [43] reported that increasing T_{in} in a CH_4 /air micro-channel combustor leads to an increase in the external wall temperature, accompanied by an upstream shift of the high-temperature region. However, the present study exhibits a different trend, where both the wall-averaged temperature and wall heat loss decrease with increasing T_{in} . This discrepancy is mainly attributed to the distinct flame structural evolution in the present combustor. As discussed above, the upstream shift and axial compaction of the reaction zone shorten the effective wall-heating length, thereby weakening the cumulative wall-heating effect and leading to a lower wall-averaged temperature.

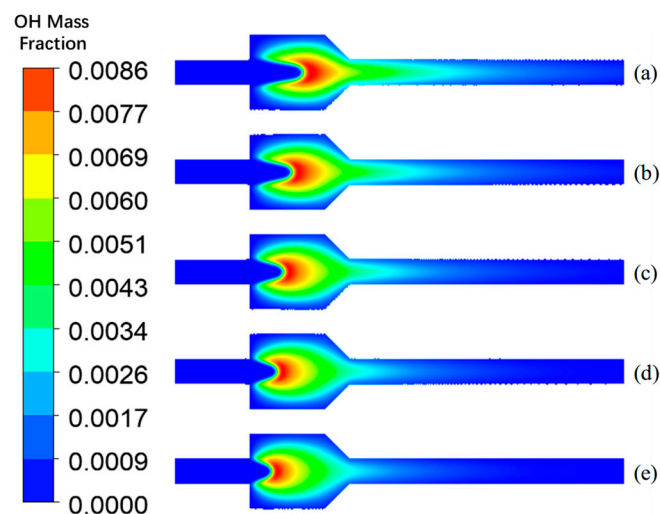


Figure 13. OH radical distributions at different T_{in} : (a) $T_{in} = 300$ K, (b) $T_{in} = 350$ K, (c) $T_{in} = 400$ K, (d) $T_{in} = 450$ K, (e) $T_{in} = 500$ K.

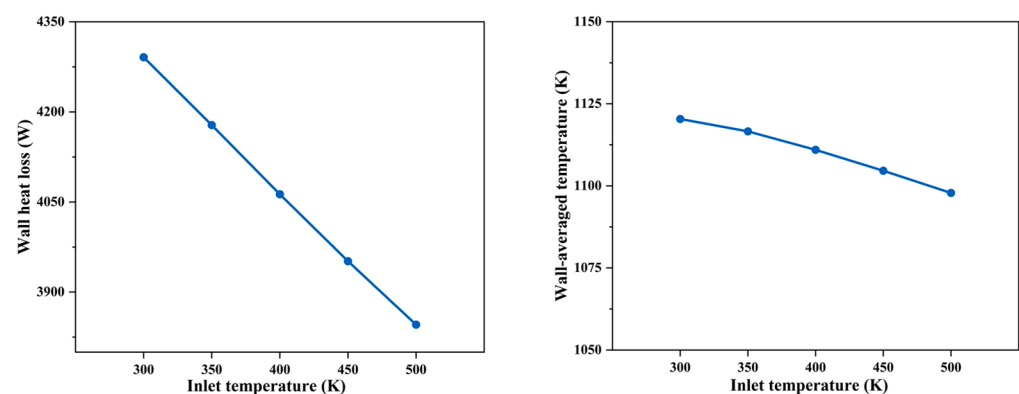


Figure 14. Wall heat loss and wall-averaged temperature at different T_{in} .

Figure 15 illustrates the pronounced influence of inlet temperature on NO formation, evidenced by both a substantial increase in NO concentration and an upstream shift of the high-NO region. At low T_{in} , the high-NO zone is largely confined to the trailing edge of the cavity and the downstream region, with relatively low intensity and limited spatial extent. In contrast, as T_{in} increases to 500 K, the high-NO region becomes significantly more intense and emerges earlier within the cavity, closely aligning with the high-temperature reaction zone. The elevated inlet temperature accelerates the preheating of the incoming mixture, promoting the decomposition of NH_3 via H-abstraction reactions (e.g., R3:

$\text{NH}_3 + \text{O} = \text{NH}_2 + \text{OH}$). Crucially, the higher local temperatures significantly enhance the chain-branching reaction ($\text{H} + \text{O}_2 = \text{O} + \text{OH}$), resulting in an enriched pool of O and OH radicals. This radical abundance shifts the consumption of amine intermediates (NH_i) towards oxidation pathways. Specifically, the contribution of reaction R5 ($\text{NH} + \text{O} = \text{NO} + \text{H}$) increases markedly, becoming the dominant route for fuel-NO formation. This kinetic shift favors direct NO production over recombination pathways, leading to the observed intensification of NO emissions. Additionally, the higher local temperatures accelerate overall reaction kinetics, further increasing the conversion of fuel-bound nitrogen to NO. As a result, the high-NO zone not only intensifies but also shifts upstream, as shown in Figure 15, reflecting a more rapid and spatially concentrated NO production process driven by inlet preheating. Cai et al. [42] also reported that increasing T_{in} reduces both the outer-wall mean temperature and the NO concentration in an NH_3/O_2 micro-planar combustor, which is partially consistent with the present thermal-response trend. However, the opposite NO trend observed in the present work highlights the strong sensitivity of NO formation to oxidizer composition and fuel chemistry in microscale combustion systems. The discrepancy arises from the different controlling mechanisms governing wall thermal response and NO formation. In the present partially cracked $\text{NH}_3/\text{H}_2/\text{N}_2$ cavity combustor, increasing T_{in} shifts and compresses the reaction zone upstream, thereby shortening the effective wall-heating length and reducing the wall-averaged temperature and heat loss. Nevertheless, this structural compaction simultaneously intensifies the localized high-temperature reaction zone and enriches the O and OH radical pool, which promotes the oxidation of fuel-bound nitrogen to NO. Therefore, while the integrated wall-heating effect is weakened, the localized high-temperature chemistry favors enhanced NO formation, leading to the distinct NO response compared with Cai et al.

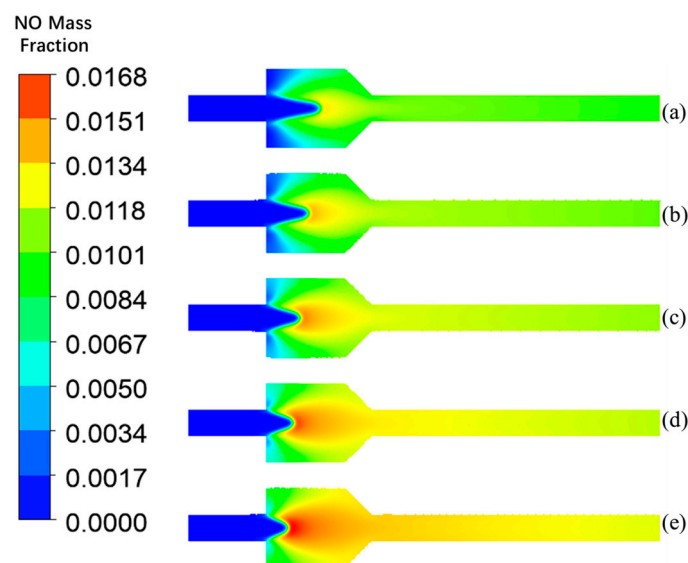


Figure 15. NO radical distributions at different T_{in} : (a) $T_{\text{in}} = 300$ K, (b) $T_{\text{in}} = 350$ K, (c) $T_{\text{in}} = 400$ K, (d) $T_{\text{in}} = 450$ K, (e) $T_{\text{in}} = 500$ K.

As shown in Figure 16, increasing T_{in} from 300 K to 500 K leads to a monotonic decrease in outlet NO_2 concentration, while N_2O emissions increase gradually. Under elevated inlet temperature conditions, the high-temperature reaction zone shifts upstream and becomes axially compressed, leading to accelerated NH_3 decomposition and enhanced formation of nitrogenous intermediates (NH_i), which serve as precursors for N_2O generation. At the same time, the compression of the intense reaction zone effectively extends the downstream post-flame region, creating a longer low-temperature environment. In this

extended post-flame zone, the thermal decomposition and further oxidation of N_2O are limited, allowing a larger fraction of N_2O to persist and exit the combustor. Consequently, the enhanced N_2O formation in the concentrated high-temperature region, combined with limited decomposition in the extended low-temperature post-flame zone, leads to increased outlet N_2O emissions with rising T_{in} .

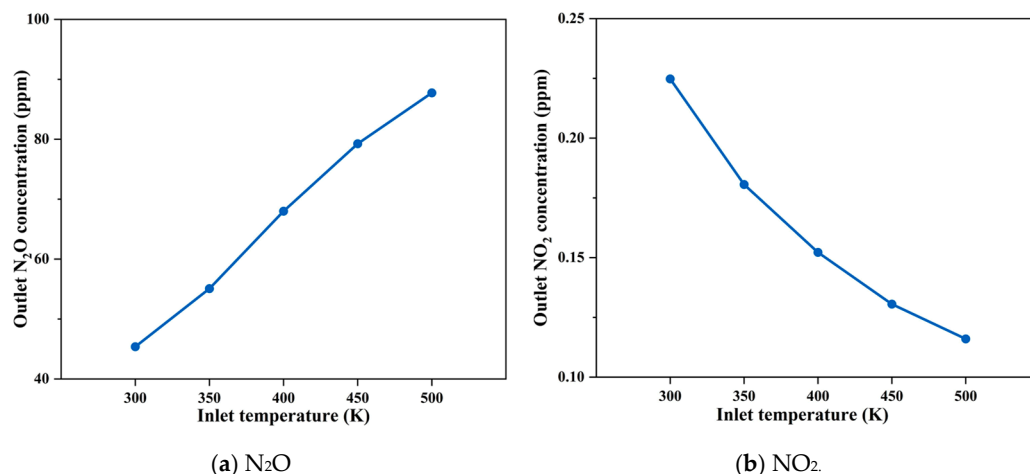


Figure 16. Outlet concentrations of N_2O and NO_2 at different T_{in} .

In contrast, the formation and evolution of NO_2 under elevated T_{in} are also governed by both the upstream compression of the intense reaction zone and the extended post-flame region, but through distinct kinetic pathways. In the concentrated high-temperature zone, the formation of NO is significantly promoted, while the generated NO_2 in the same region is prone to thermal decomposition, thereby suppressing its accumulation. The compression of this high-temperature region further reduces the spatial domain where radical-driven NO oxidation can occur, thereby decreasing overall NO_2 formation. Additionally, although the post-flame region is extended, the lower temperatures and depleted concentrations of oxidizing radicals in this zone still restrict the secondary conversion of NO to NO_2 . Consequently, the combined effects of upstream thermal decomposition, reduced high-temperature reaction space and limited low-temperature oxidation contribute to the decrease in outlet NO_2 concentrations under elevated inlet temperature conditions, exhibiting an opposite trend to that observed for N_2O emissions. These observations highlight the contrasting sensitivity of different nitrogen oxides to changes in reaction zone structure and post-flame environment under elevated T_{in} conditions.

4. Conclusions

This study systematically investigates the combustion and emission characteristics of premixed partially cracked NH_3 /air flames in a cavity micro-combustor, focusing on the effects of equivalence ratio (Φ) and inlet temperature (T_{in}) on the temperature field, OH radical concentrations, wall heat loss and pollutant emissions. The results obtained are summarized as follows:

Increasing the equivalence ratio from $\Phi = 0.8$ to 1.2 shifts the high-temperature region downstream and elongates it axially due to the prolonged fuel oxidation process under oxygen-deficient conditions, resulting in a lower peak temperature and more distributed heat release. The mean wall temperature and overall heat loss are thus decreased at $\Phi = 1.2$, reflecting a weakened high-temperature reaction zone near the cavity and reduced near-wall thermal interaction. NO formation closely follows the high-temperature and OH -rich zones. Specifically, at $\Phi = 0.8$, NO production is dominated by fuel-nitrogen chemistry driven by abundant radicals. At $\Phi = 1.2$, NO formation is suppressed as the scarcity of

O and OH radicals inhibits the oxidation of amine intermediates (e.g., $\text{NH}/\text{NH}_2 \rightarrow \text{NO}$). Under these fuel-rich conditions, the diminished oxidation environment also redirects fuel-bound nitrogen toward N_2O , enhancing its accumulation at the combustor outlet. While fuel-rich operation ($\Phi = 1.2$) effectively minimizes NO emissions, it compromises flame stability by shifting the reaction zone downstream, suggesting the need for thermal enhancement to ensure robust anchoring.

Increasing the inlet temperature from 300 K to 500 K enhances the reactivity of the mixture by promoting chain-branching reactions and enriching the O/OH radical pool, advancing the formation of the main reaction zone and concentrating it in the cavity. This upstream shift not only elevates NO production but also compresses the high-temperature zone axially. The resulting shorter heated length reduces the wall-averaged temperature and the overall convective and radiative heat loss, despite the locally higher peak temperatures. The extended downstream post-flame region, characterized by lower temperatures and limited radical activity, restricts NO_2 formation and N_2O decomposition. Hence, the outlet NO_2 concentrations decrease monotonically with increasing T_{in} , while N_2O emissions exhibit a rising trend. Although high inlet temperatures lead to increased NO emissions, they are essential for minimizing heat loss and stabilizing the flame. Therefore, an operating strategy combining fuel-rich conditions ($\Phi = 1.2$) with elevated inlet temperatures ($T_{\text{in}} = 500$ K) is suggested as the optimal choice. This approach leverages oxygen deficiency to mitigate NO formation while utilizing inlet preheating to ensure robust combustion stability.

In addition, comparisons with representative microscale CH_4 -, H_2 - and NH_3 -fueled combustion studies suggest that several trends identified herein reflect intrinsic characteristics of confined micro-combustion systems. In particular, the spatial distribution and structural evolution of the reaction zone play a critical role in governing both wall thermal response and pollutant formation, exhibiting strong sensitivity to equivalence ratio and inlet temperature. Nevertheless, the partially cracked $\text{NH}_3/\text{H}_2/\text{N}_2$ -air cavity combustor exhibits pronounced fuel-specific behavior, particularly in the transformation pathways of nitrogen-containing species. The coupling between heat release and NO formation is fundamentally modulated by fuel-nitrogen chemistry, NH_3 reburning processes and the dilution effect associated with cracking-generated N_2 . These interacting mechanisms alter the interplay between localized high-temperature radical kinetics and the integrated wall-heating response. Accordingly, although the qualitative flame-wall thermal coupling behavior may be broadly applicable across different fuels, direct quantitative extrapolation of emission characteristics from CH_4 or H_2 systems to partially cracked ammonia flames should be undertaken with caution. Future investigations should emphasize systematic cross-fuel comparisons under matched geometrical configurations and boundary conditions, with particular focus on reaction-zone redistribution and fuel-nitrogen conversion pathways.

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