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Numerical Investigation of Combustor Inlet Temperature Effects on Emissions and Performance in Non-Premixed Ammonia-Fueled Micro-Gas Turbines

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Abstract

Ammonia combustion is emerging as a carbon-free energy solution, offering the potential to lower greenhouse gas emissions. Its role as a green hydrogen carrier makes it suitable for use in hard-to-abate sectors as a renewable fuel. However, its combustion produces high NO_x emissions due to the nitrogen content in the fuel molecule, especially under lean conditions at elevated air temperatures, as in gas turbine combustors.

In this study, a detailed CFD-based numerical investigation of an optimized 20-kW staged rich-lean ammonia-fueled, non-premixed combustion chamber was carried out to investigate the effects of combustor inlet temperature (CIT) on emissions, combustion efficiency, and overall performance. The CIT was increased from 500 K to 1050 K at a $\phi_{overall}$ of 0.12. This temperature rise resulted in a 430 K increase in combustor outlet temperature (COT), from 860 K to 1300 K, and a 50% rise in NO_x emissions from 308 to

627 ppm. The higher COT, combined with reductions in unburned NH_3 and H_2 by 90% (1094 to 101 ppm) and 27% (0.03 to 0.02 Vol.%), respectively, contributed to a 5% improvement in combustion chamber efficiency based on output power.

This CFD-based study also integrates the effects of CIT and different $\phi_{overall}$ (0.12 to 1.2) to comprehensively assess the factors influencing combustion efficiency and emissions. The findings provide simulation-driven insights to optimize performance, reduce emissions, and guide the design of future ammonia-fueled micro gas turbines.

Keywords: Ammonia Combustion, Micro Gas Turbine, Combustion Efficiency, CIT, Emissions.

Nomenclature

χ Scalar Dissipation Rate ($\frac{1}{s}$)

$\dot{\omega}$ Chemical Source Term ($\frac{kg}{m^2s}$)

$\dot{m}_{air}$ Air Mass Flow Rate ($\frac{kg}{s}$)

$\dot{m}_{fuel}$ Fuel Mass Flow Rate ($\frac{kg}{s}$)

μ Molecular Viscosity ($\frac{kg}{ms}$)

ν Kinematic Viscosity ($\frac{m^2}{s}$)

$\phi_{overall}$ Overall Equivalence Ratio

39	$\phi_{primary}$	Primary Equivalence Ratio
40	ρ	Density ($\frac{kg}{m^3}$)
41	σ	Turbulent Prandtl Number
42	ε	Dissipation Rate of Turbulent Kinetic Energy ($\frac{m^2}{s^3}$)
43	D	Molecular Diffusivity ($\frac{m^2}{s}$)
44	Da	Damköhler Number
45	G	Generation of Turbulent Kinetic Energy ($\frac{m^2}{s^3}$)
46	k	Turbulent Kinetic Energy ($\frac{m^2}{s^2}$)
47	S	Modulus of the Mean Strain Rate ($\frac{1}{s}$)
48	u_j	Velocity Component ($\frac{m}{s}$)
49	Y	Mass Fraction
50	Z	Mixture Fraction
51	CFD	Computational Fluid Dynamics
52	CH₄	Methane
53	CIT	Combustor Inlet Temperature
54	CNG	Compressed Natural Gas
55	CO₂	Carbon Dioxide

56 **COT** Combustor Outlet Temperature

57 **CO** Carbon Monoxide

58 **GHG** Greenhouse Gases

59 **GT** Gas Turbine

60 **H₂O** Water

61 **H₂** Hydrogen

62 **LHV** Lower Heating Value ($\frac{MJ}{kg}$)

63 **LNG** Liquefied Natural Gas

64 **mGT** Micro Gas Turbine

65 **N₂** Nitrogen

66 **NG** Natural Gas

67 **NH₃** Ammonia

68 **NO_x** Nitrogen Oxides

69 **NO** Nitrogen Monoxide

70 **Power_{th}** Thermal Power (kW)

71 **SCR** Selective Catalytic Reduction

72 1. Introduction

73 Combustion plays a key role in industrial sectors such as power genera-
74 tion, transportation, and manufacturing. Currently, fossil fuel combustion
75 supplies about 80% of global electricity demand [1], but it is also a major
76 source of carbon emissions like CO and CO₂, which contribute significantly
77 to climate change. Despite efforts to improve efficiency and reduce GHG
78 emissions, such measures alone are insufficient to meet decarbonization tar-
79 gets [2]. Achieving environmental goals requires adopting renewable and
80 low-carbon fuels [3]. However, renewable energy faces challenges such as in-
81 termittency, limited storage capacity, and high infrastructure costs [4], while
82 many industrial applications still rely on combustion to achieve high process
83 temperatures.

84 Hydrogen is a promising alternative to fossil fuels due to its high energy
85 density and near-zero CO₂ emissions. However, its large-scale adoption is
86 constrained by production costs and the need for new storage and distribution
87 infrastructure [5].

88 Ammonia has emerged as a promising carbon-free fuel with high hydro-
89 gen content (17.8% by mass) [6], low storage costs, and compatibility with
90 existing infrastructure [7]. It offers higher volumetric energy density than hy-
91 drogen and benefits from established transport and storage protocols, making
92 it especially suitable for long-term and large-scale applications [5]. However,
93 ammonia presents combustion challenges due to its low laminar burning ve-
94 locity (≈ 7 cm/s under stoichiometric conditions at 300 K and 0.1 MPa),

95 which can lead to flame instability and reduced reactivity [8, 9]. In addition,
96 ammonia combustion is associated with high NO_x emissions due to its high
97 nitrogen content, requiring advanced strategies to mitigate environmental
98 impacts [10].

99 Ammonia can be utilized either by cracking into hydrogen and nitrogen
100 [11] or directly as a zero-carbon fuel in power generation systems. Recent
101 developments have shown that direct use in fuel cells and gas turbines is fea-
102 sible, although combustion-related challenges persist [12, 2]. Ammonia-based
103 power generation using renewable or nuclear-derived ammonia can achieve a
104 near-zero carbon footprint, particularly when waste heat is recovered [13].

105 To build on ammonia’s potential, gas turbines (GTs) represent a criti-
106 cal technology for carbon-free power generation [14]. GTs are widely used
107 in industrial applications due to their efficiency, scalability, and operational
108 flexibility. Among them, micro gas turbines (mGTs) have gained attention
109 for their compact size and high reliability. Operating typically in the 1–500
110 kW range [15], mGTs are well suited for decentralized energy systems and
111 testing alternative fuels such as ammonia. Their modularity and adaptabil-
112 ity make them excellent platforms for developing and validating ammonia
113 combustion concepts [16].

114 Several studies have explored ammonia-fueled gas turbines through both
115 thermodynamic and experimental approaches. Keller et al. [17] proposed a
116 combined-cycle system with exhaust gas recirculation (EGR), while Ayaz et
117 al. [18] analyzed a Turbec T100 mGT with ammonia blends, showing that

118 higher ammonia content reduced efficiency. Bonasio et al. [19] confirmed the
119 feasibility of direct ammonia combustion in a 100-kW mGT. Božo and Valera-
120 Medina [20] demonstrated that a humidified ammonia/hydrogen Brayton
121 cycle can reach efficiencies comparable to fossil fuel systems.

122 In our previous work [21], we simulated a 3 kW mGT using ammonia fuel,
123 showing comparable power output to methane with slightly lower efficiency
124 (5.16%). We later investigated steam injection [22], which improved efficiency
125 and reduced NO_x emissions by 36%, highlighting the potential of combined
126 strategies for performance enhancement.

127 Hydrogen addition has been widely investigated to overcome ammonia's
128 low reactivity. Its high flame speed and reactivity improve stability and ex-
129 pand the flammability range. Catalytic cracking can generate hydrogen in
130 situ, further enhancing flame stability [23]. Studies show that with a hydro-
131 gen fraction of 0.4, the laminar burning velocity approaches typical hydrocar-
132 bon flames [24], and blends near 50:50 yield methane-like flame speeds [25].
133 However, hydrogen's high diffusivity can increase flashback risk, requiring
134 careful burner design.

135 Recent experimental works also examined the effects of hydrogen fraction
136 on stability and emissions. Franco et al. [26] and Pacheco et al. [27] reported
137 that moderate H_2 additions enhance flame stability and lower NO_x . Li et
138 al. [28] further highlighted that optimized H_2 - NH_3 ratios improve engine
139 efficiency and reduce misfiring.

140 Compared to pure ammonia, NH_3 - CH_4 blends improve ignition and flame

141 stability while emitting less CO_2 than pure CH_4 [29]. However, methane ad-
142 dition can also increase CO and NO_x at higher CH_4 ratios [30, 31]. Although
143 promising, such blends still require optimization to control emissions.

144 Pure NH_3 combustion has also been extensively studied. Hayakawa et al.
145 [33] demonstrated stable premixed ammonia/air flames in a swirl combustor,
146 while Okafor et al. [34] showed that rich-lean staging reduces emissions
147 in liquid ammonia spray systems. These findings underline the need for
148 improved flame control and staging strategies for practical GT applications.

149 Because of the significant NO_x emissions from NH_3 combustion, many
150 studies have focused on mitigation. Staged combustion, optimized equiv-
151 alence ratios, and selective catalytic reduction (SCR) are among the most
152 effective techniques [35, 36]. SCR converts NO_x into N_2 and H_2O using am-
153 monia or urea in the presence of a catalyst, achieving high efficiency and
154 reliability [37]. Integrating SCR with optimized combustion conditions can
155 further improve NO_x control.

156 Experimental and numerical studies have focused on combustor optimiza-
157 tion for NO_x reduction. Okafor et al. [38] demonstrated that inclined injec-
158 tion and a two-stage rich-lean strategy reduced NO_x to 42 ppmv. Ni et al.
159 [39] showed that a double-rib structure in micro-combustors improved ther-
160 mal performance and reduced NO emissions by 47%. Somarathne et al. [40]
161 found that increased pressure in premixed NH_3 /air flames lowered NO and
162 unburned NH_3 , while Kurata et al. [41] developed a non-premixed rich-lean
163 combustor with one-third lower NO emissions. Wang et al. [42] numeri-

164 cally investigated NH_3 /air flames using flamelet models, highlighting lower
165 NO_x formation under mGT conditions. In our recent work [43], a redesigned
166 staged combustor with $\phi_{primary}=1.07$ reduced NO by two-thirds compared to
167 the baseline case.

168 This study investigates the effect of combustor inlet temperature (CIT)
169 on emissions, temperature, and combustion efficiency through detailed CFD
170 simulations. The role of unburned NH_3 and H_2 was also analyzed to evaluate
171 combustion completeness and flame stability. Although the effect of CIT
172 has been explored in previous works [36], most studies focused on global
173 combustion behavior rather than emissions in mGT-scale combustors.

174 The case examined here builds on a previously optimized combustor ge-
175 ometry [43], confirming its suitability for ammonia combustion at specific
176 equivalence ratios and CIT. Micro gas turbines often employ regenerators to
177 increase CIT and efficiency [44]; however, the influence of varying CIT on
178 emissions and flame stability remains insufficiently characterized.

179 The novelty of this study lies in providing an in-depth analysis of CIT
180 effects on NO_x , unburned fuel, and stability in a non-premixed rich-lean
181 mGT combustor. By jointly examining CIT and global equivalence ratio,
182 this work offers integrated insights to support the design of next-generation
183 low-emission ammonia turbines.

184 2. Methodology

185 The MTT-EnerTwin is a compact recuperated micro gas turbine (mGT)
186 featuring the combustor analyzed in this study. It achieves an electrical
187 efficiency of 16% and generates 3.2 kW_e of power, with a maximum rotational
188 speed of 240,000 rpm. The combustor was originally designed to operate on
189 hydrocarbon fuels such as methane, NG, LNG, and CNG. Moreover, it can
190 run on hydrocarbon fuel blends containing up to 23% hydrogen. In our
191 previous work [43], the combustor was redesigned and optimized for burning
192 ammonia based on the rich-lean combustion strategy.

193 2.1. Combustion chamber geometry and boundary conditions

194 Combustion takes place in a straight-flow, non-premixed can-typed com-
195 bustor operating in a rich regime ($\phi_{primary} = 1.07$) within the primary zone,
196 with an overall equivalence ratio ($\phi_{overall}$) of 0.12. Figure 1 illustrates the
197 design parameters and structure of the optimized combustion chamber con-
198 figured for ammonia fueling in the mGT. Based on results from a simple
199 cold-flow CFD simulation, 12% of the air enters the inner liner, supplying
200 the primary combustion zone after passing through the swirler [43]. The
201 remaining air flows into the outer liner and subsequently feeds other zones
202 via primary cooling sleeves, 16 dilution holes, secondary cooling sleeves, and
203 the gaps between the inner and outer liners near the outlet.

204 According to our previous study [21], the optimal operating conditions
205 for the mGT cycle include a nominal rotational speed of 240,000 rpm, a

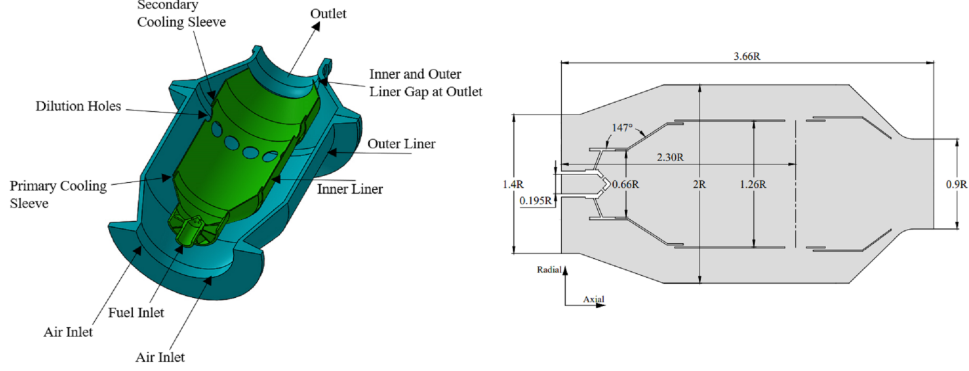


Figure 1: Three-dimensional model of the non-premixed swirl combustion chamber and the dimensions of its central cross-section (computational domain)

206 fuel mass flow rate of 1.13 g/s, a fuel inlet temperature of 300 K, an air
 207 mass flow rate of 0.055 kg/s, an air inlet temperature of 1050 K, and an
 208 operating pressure of 3.0 bar. Building on this, the present study varied the
 209 air inlet temperature from 500 K to 1050 K (specifically 500 K, 600 K, 700
 210 K, 800 K, 900 K, and 1050 K) to analyze its effects on emissions, efficiency,
 211 and combustion stability within the chamber while keeping the fuel inlet
 212 temperature fixed at 300 K. Table 1 presents the air and fuel mass flow rates
 213 corresponding to different overall equivalence ratios, with the calculations
 214 based on a constant thermal power of 20 kW. To address the reduced outlet
 215 temperatures associated with lower air inlet temperatures, a range of overall
 216 equivalence ratios was investigated to maintain sufficient outlet temperature
 217 levels. The fuel and air mass flow rates have been calculated according to the
 218 LHV of ammonia (18.6 MJ/kg) and the required heat input, and the overall
 219 equivalence ratio according to Equations 1, 2.

$$\dot{m}_{fuel} = \frac{\text{Power}_{th}}{\text{LHV}_{fuel}} \quad (1)$$

$$\dot{m}_{air} = \dot{m}_{fuel} * \frac{6.05}{\phi_{overall}} \quad (2)$$

Where $\dot{m}_{fuel}$ is the mass flow rate, Power_{th} is the required thermal power, LHV_{fuel} is the lower heating value of the fuel, $\dot{m}_{air}$ is the air mass flow rate, $\phi_{overall}$ is the overall equivalence ratio of the combustion, and 6.05 is the stoichiometric equivalence ratio of burning ammonia with air based on Equation 3.

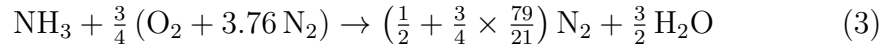


Figure 2 illustrates the airflow and fuel distribution within the combustion chamber, highlighting the division into the primary zone and the dilution zone. Fuel is injected into the primary zone along with a portion of the total air, referred to as primary air, which initiates the combustion process. The remaining airflow is introduced downstream through secondary and dilution ports, labeled as Air 1, Air 2, and Air 3, to control flame temperature, complete combustion, and reduce NO_x emissions.

The total air mass flow rate ($\dot{m}_{air}$) entering the combustor is therefore composed of the primary air and the staged airflows introduced in the dilution zone. This is expressed in Equation 4:

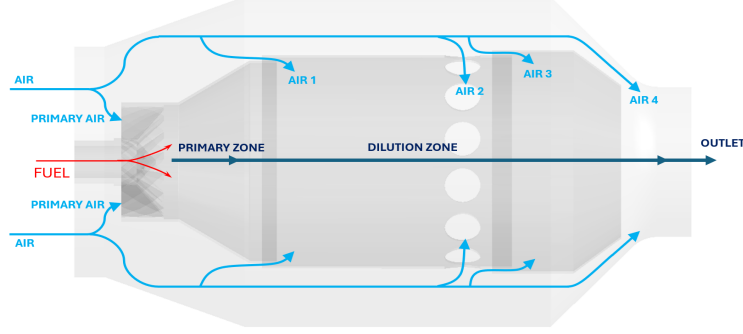


Figure 2: Configuration of airflow and fuel distribution within the combustion chamber

$$\dot{m}_{air} = \dot{m}_{PrimaryAir} + \dot{m}_{Air1} + \dot{m}_{Air2} + \dot{m}_{Air3} + \dot{m}_{Air4} \quad (4)$$

235 To characterize the combustion conditions specifically in the primary
 236 zone, the $\phi_{primary}$ is defined as the ratio of fuel mass flow rate to the mass
 237 flow rate of the primary air, normalized by the stoichiometric air-to-fuel mass
 238 ratio of ammonia (6.05). This is calculated using Equation 5:

$$\phi_{primary} = \frac{6.05 \times \dot{m}_{fuel}}{\dot{m}_{PrimaryAir}} \quad (5)$$

239 This parameter is crucial in analyzing local flame behavior, ignition sta-
 240 bility, and pollutant formation within the primary combustion zone.

241 2.2. Turbulence and combustion model

242 A realizable RANS $k - \varepsilon$ model was used. The transport equations for
 243 turbulent kinetic energy and dissipation rate are solved using two equations,
 244 which form the foundation of the model [45]. Unlike the standard $k - \varepsilon$

Table 1: Fuel and air mass flow rates for different $\phi_{overall}$.

$\phi_{overall}$	$\dot{m}_{fuel}$ (kg/s)	$\dot{m}_{air}$ (kg/s)
0.12	0.00107	0.0551
0.3	0.00107	0.0210
0.6	0.00107	0.0108
0.8	0.00107	0.0080
1.0	0.00107	0.0065
1.1	0.00107	0.0059
1.2	0.00107	0.0054

245 model, it introduces a new approach to turbulent viscosity and a novel dis-
 246 sipation rate transport equation, ε , derived from an exact equation for the
 247 mean-square vorticity fluctuation. The realizable $k - \varepsilon$ model is a widely
 248 used turbulence model that provides improved predictions for a variety of
 249 flows, particularly those involving strong curvature, rotation, and separated
 250 flows. Combustion processes, especially in non-premixed flames, rely heavily
 251 on the turbulent mixing of fuel and oxidizer. The realizable $k-\varepsilon$ model's
 252 enhanced capabilities in capturing turbulence effects lead to more accurate
 253 representations of mixing, which directly impacts the combustion process.
 254 Moreover, the model's ability to handle flows with strong curvature and sep-
 255 aration points makes it suitable for combustion applications.

256 Equation 6 shows the transport equation for k :

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho k u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k - \rho \varepsilon, \quad (6)$$

257 Where ρ is the fluid density, u_j is the velocity component, μ is the molecu-
 258 lar viscosity, μ_t is the turbulent viscosity, σ_k is the turbulent Prandtl number

259 for k , G_k represents the generation of turbulent kinetic energy due to mean
 260 velocity gradient, and ε is the dissipation rate of k .

261 The transport equation ε is indicated as Equation 7:

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \frac{\partial(\rho\varepsilon u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_1 S \varepsilon - C_2 \frac{\rho \varepsilon^2}{k + \sqrt{\nu \varepsilon}}, \quad (7)$$

262 where σ_ε is the turbulent Prandtl number for ε , C_1 and C_2 are model
 263 constants, S is the modulus of the mean strain rate, and ν is the kinematic
 264 viscosity.

265 The turbulent viscosity μ_t is calculated as Equation 8:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon}, \quad (8)$$

266 The key distinction between the realizable $k - \varepsilon$ model and the standard
 267 and RNG $k - \varepsilon$ models is that C_μ is not treated as a constant in the realizable
 268 model. It is a function of the mean strain and rotation rates, the angular
 269 velocity of the system rotation, and the turbulence fields (k and ε) [45, 46].

270 The steady flamelet model from diffusion flamelet theory has been used
 271 for the combustion model. Turbulent, non-premixed flames are commonly
 272 characterized by the Damköhler number (Da), which represents the ratio of
 273 the mixing timescale to the chemical reaction timescale. When $Da \gg 1$,
 274 chemical reactions occur rapidly enough to prevent fuel from penetrating the
 275 reaction zone to the oxidizer side and vice versa. The Damköhler number

276 plays a crucial role in the rapid chemical reactions of non-premixed combus-
 277 tion processes in practical applications [47]. In such cases, turbulent mixing
 278 controls reaction kinetics, resulting in a small chemical timescale. To model
 279 rapid chemistry and mass transfer in non-premixed combustion, the steady
 280 flamelet model derived from diffusion flamelet theory [48, 49] was employed.
 281 For a species mass fraction Y_i in mixture fraction space, the steady
 282 flamelet equation is described as Equation 9:

$$\rho \frac{\partial Y_i}{\partial t} = 0 = \rho \frac{\chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} + \dot{\omega}_i, \quad (9)$$

283 Where ρ is density, Y_i is the mass fraction of species i , Z is mixture
 284 fraction (ranges from 0 to 1), χ is scalar dissipation rate. It is defined as
 285 Equation 10 with D_z as the molecular diffusivity of Z :

$$\chi = 2D_z \left(\frac{\partial Z}{\partial x_j} \frac{\partial Z}{\partial x_j} \right) \quad (10)$$

286 and $\dot{\omega}_i$ is the chemical source term of species i .

287 According to the flamelet concept, a turbulent flame comprises thin, spa-
 288 tially one-dimensional, laminar flamelet structures embedded within the tur-
 289 bulent flow. A counterflow diffusion flame is typically used to represent a
 290 flamelet in turbulent flows. In this setup, the fuel and oxidizer jets are ar-
 291 ranged oppositely and symmetrically along an axis. As the distance between
 292 the jets decreases and their velocity increases, the flame is strained and moves
 293 away from chemical equilibrium, eventually extinguishing. The mixture frac-

tion [48] in the laminar counterflow flame decreases monotonically from unity
 at the fuel jet to zero at the oxidizer jet [46]. By mapping the physical space
 to mixture fraction space, two parameters, the mixture fraction and scalar
 dissipation can uniquely describe the temperature and species mass fractions
 along the axis [48]. In this study, 10 flamelets were considered, each with 64
 grid points. Although this configuration increased solution time and mem-
 ory usage, it provided higher resolution and greater accuracy in predicting
 species formation. Moreover, this configuration was adopted based on our
 previous work [43], where we introduced and validated the current combus-
 tion chamber geometry through CFD simulations for ammonia combustion.
 In that study, the same number of flamelets was shown to accurately capture
 key flame characteristics while ensuring computational efficiency. To ensure
 consistency and comparability with the validated setup, the same resolution
 has been used in the present investigation.

Several chemical kinetic mechanisms have been proposed in the litera-
 ture for ammonia (NH_3) oxidation; however, their applicability often varies
 with pressure, temperature, and equivalence ratio [51]. In this study, the
 optimized kinetic mechanism developed by Stagni et al. [52] is employed. It
 includes 31 species and 203 reactions and was specifically designed for com-
 bustion modeling. The mechanism has been experimentally validated against
 a broad set of conditions, accurately capturing key features of ammonia ox-
 idation, NO production, and reburn chemistry over a wide operating enve-
 lope. Its proven reliability ensures that the present predictions of ammonia

317 combustion behavior, including NO formation pathways, are robust.

318 Direct experimental validation of the present study conditions is not avail-
319 able; however, the overall emission trends predicted in this study are in good
320 agreement with the experimental work of Kurata et al. [36]. Their mea-
321 surements demonstrated that increasing combustor inlet temperature (CIT)
322 promotes higher NO formation while simultaneously reducing unburned NH_3 ,
323 as enhanced reaction rates improve fuel conversion. The same behavior is
324 observed in the present CFD results, where NO exhibits an increasing trend
325 and NH_3 a decreasing trend with rising CIT. This consistency supports the
326 credibility of the numerical predictions. It is also worth noting that while
327 Kurata et al. explored CIT values up to 800 K without considering differ-
328 ent equivalence ratios, the present study extends the analysis to 1050 K and
329 systematically investigates a range of equivalence ratios. This broader oper-
330 ating window provides additional insights into the combustion characteristics
331 of ammonia under conditions relevant to gas turbine applications.

332 *2.3. Computational mesh*

333 A mesh sensitivity analysis was conducted to identify the geometric re-
334 gions requiring mesh refinement. The primary combustion zone, dilution
335 holes, and swirler zone emerged as the most critical areas due to the presence
336 of higher gradients in fluid dynamics and thermal properties. A tetrahedral
337 grid network consisting of approximately 8 million cells was generated for all
338 cases using ANSYS MESH[®]. Figure 3a illustrates the mesh configuration.

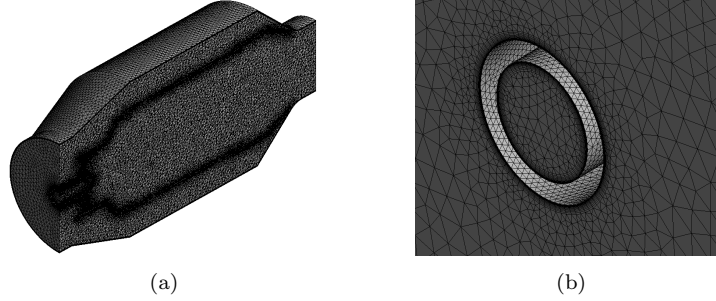


Figure 3: Mesh configuration (a) computational Mesh of the fluid domain, (b) inflation in the inlet area of the fuel injector

339 Additional refinement was applied near the wall regions using the inflation
 340 option, with the first element height set to 1×10^{-5} m, a growth rate of 1.2,
 341 and 15 layers above the wall. The maximum y^+ value obtained during the
 342 simulations was 1.47, observed in the swirler zone, aligning with the recom-
 343 mended values for accurately capturing the primary fluid dynamic features
 344 of the turbulence model described in [46]. Figure 3b depicts the 15-layer
 345 inflation setup.

346 In this study, three different mesh configurations, ranging from 4 to 12
 347 million cells, were utilized to evaluate the influence of mesh resolution on
 348 simulation accuracy. The primary aim of the mesh sensitivity analysis was
 349 to ensure that the computational grid was sufficiently refined to capture
 350 essential flow and combustion characteristics while avoiding excessive com-
 351 putational costs. Figure 4 illustrates the temperature distribution along the
 352 combustor centerline for case 5, allowing a visual comparison of results from
 353 each mesh configuration. The figure reveals that the temperature profiles
 354 obtained with 8 million and 12 million cells are nearly identical, indicating

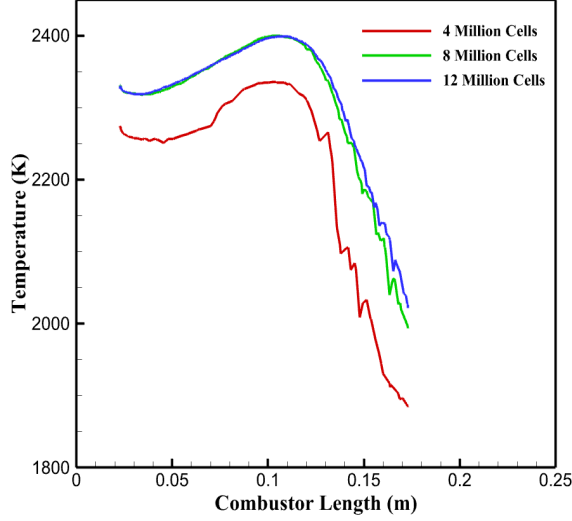


Figure 4: Grid independence validation via temperature along the combustor length

355 that the solution has converged at this level of mesh refinement. This con-
 356 vergence demonstrates that increasing the cell count beyond 8 million does
 357 not significantly enhance accuracy, as the computational results have already
 358 stabilized.

359 2.4. Computational setup

360 The combustion process was simulated in 42 cases using computational
 361 fluid dynamics (CFD) methods, considering seven overall equivalence ratios
 362 (Table 1) and six different CITs (500 K, 600 K, 700 K, 800 K, 900 K, and
 363 1050 K). The simulations were performed with the commercial software AN-
 364 SYS FLUENT[®] on a scalar supercomputer equipped with 64 CPUs (AMD
 365 EPYC 7501 32) and 512 GB of RAM. Each simulation, including the bound-
 366 ary conditions, required approximately one hour of computation time. This

relatively short solution time is notable given the substantial computational demands of combustion simulations, which necessitate solving a large system of coupled nonlinear equations governing fluid dynamics, heat transfer, chemical reactions, and turbulence. The computational efficiency of the simulation process allowed for the exploration of numerous scenarios and configurations within a practical time frame, enabling a comprehensive analysis of combustion dynamics and emission characteristics across a range of operating conditions.

3. Results and discussion

This section presents the key findings of the study, focusing on the effects of combustor operating conditions on temperature and emission characteristics. The analysis highlights how variations in equivalence ratio and inlet temperature influence combustion performance and pollutant formation, providing insights relevant for optimizing gas turbine operation with ammonia-based fuels.

Figure 5 illustrates the variation of Combustor Outlet Temperature (COT) with Combustor Inlet Temperature (CIT) for different overall equivalence ratios ($\phi_{overall}$), highlighting how both parameters influence the thermal characteristics of the combustion process. The outlet temperature of the combustion gases exhibits a clear dependence on both $\phi_{overall}$ and CIT. At a fixed CIT, increasing $\phi_{overall}$ generally leads to a higher outlet temperature due to greater fuel availability and increased heat release. However, the rate of

389 temperature rise diminishes at higher $\phi_{overall}$ values, suggesting a nonlinear
390 relationship. On the other hand, for a given $\phi_{overall}$, raising the CIT results
391 in a consistent increase in outlet temperature, demonstrating the strong in-
392 fluence of initial thermal conditions on combustion. The effect of CIT is more
393 pronounced at lower $\phi_{overall}$ values, where the outlet temperature increases
394 more sharply with rising air inlet temperature.

395 At higher $\phi_{overall}$ values, particularly $\phi_{overall} = 1.0$, 1.1 , and 1.2 , the
396 outlet temperature remains significantly high across all CIT values, exceed-
397 ing 1700 K. Such conditions are far above the maximum allowable exhaust
398 temperature for gas turbine blades (≈ 1300 - 1500 K), beyond which material
399 degradation and thermal stresses become critical concerns [53, 54, 55]. In
400 addition to this thermal limitation, operation under rich conditions results
401 in incomplete combustion, leading to large amounts of unburned NH_3 in
402 the exhaust, while the elevated flame temperatures simultaneously intensify
403 NO_x formation. These effects reduce overall efficiency, increase emissions,
404 and pose significant risks to turbine integrity. For these reasons, only the
405 leaner cases ($\phi_{overall} = 0.12$ and $\phi_{overall} = 0.3$) fall within a safe and efficient
406 operating window, with $\phi_{overall} = 0.3$ remaining acceptable only when the
407 CIT is below 700 K.

408 Figure 6 indicates the temperature contour plots regarding various CIT
409 and $\phi_{overall}$ s. The top row shows the temperature distributions for $\phi_{overall} =$
410 0.12 with varying CIT values from 500 K to 1050 K, while the bottom row
411 illustrates the cases for $\phi_{overall} = 0.3$ at CIT = 500 K and 600 K. COT in these

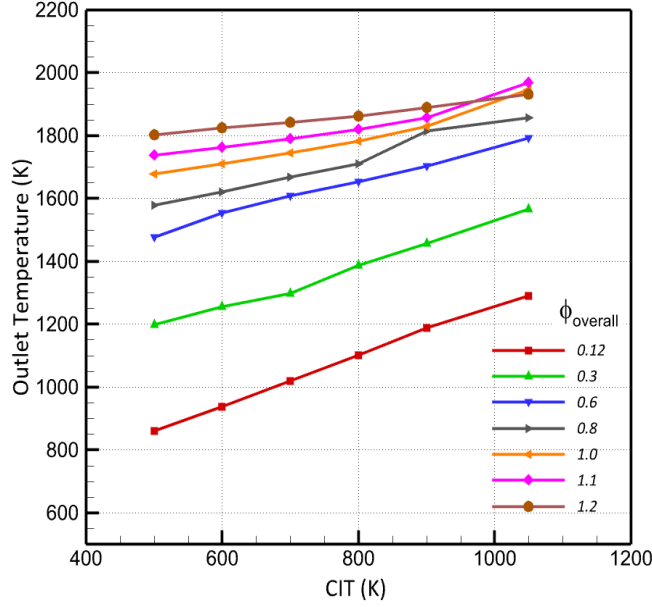


Figure 5: Combustor outlet temperature for various CITs and $\phi_{overall}$ s

cases is below the critical 1300 K threshold, suggesting that this operating
 condition is thermally viable for turbine applications. When $\phi_{overall} = 0.12$,
 the COT steadily rises as CIT increases, starting at 860 K at CIT = 500
 K and reaching 1289 K when CIT hits 1050 K. The temperature profiles
 reveal that higher inlet temperatures cause the combustion region to widen,
 making the high-temperature zones (red areas) more prominent. This pattern
 is anticipated because a higher CIT improves reaction kinetics, resulting in
 increased heat release. Conversely, the COT is substantially higher than
 the scenario with $\phi_{overall} = 0.12$. It has reached 1197 K at CIT = 500 K
 and 1255 K at CIT = 600 K. Due to the enhanced availability of fuel, the
 combustion process becomes more intense, creating a larger high-temperature
 area; additionally, there is a reduction in the dilution air mass flow rate. In

424 comparison to the combustion with $\phi_{overall} = 0.12$, the flame shape appears
425 less stable and has a more extended and uneven structure. This implies that
426 turbulence and local mixing effects have a greater influence on the flame's
427 aerodynamic properties at higher equivalence ratios, which could result in
428 flame instability. Combustion efficiency may be adversely affected by such
429 instability.

430 The concentrations of unburned NH_3 and H_2 at the outlet are key indi-
431 cators of combustion efficiency. Lower concentrations imply more complete
432 combustion, higher thermal efficiency, and reduced pollutant emissions. As
433 shown in Figures 7a and 7b, both NH_3 and H_2 concentrations consistently
434 decrease with increasing air inlet temperature (CIT) across all studied equiv-
435 alence ratios ($\phi_{overall} = 0.12, 0.3, 1.0$, and 1.2), signifying enhanced oxidation
436 and combustion completeness at higher temperatures. However, the extent
437 of unburned species varies significantly with equivalence ratio. At lean con-
438 ditions ($\phi_{overall} = 0.12$ and 0.3), the outlet concentrations of NH_3 and H_2
439 remain relatively low, with the lowest levels observed at $\phi_{overall} = 0.12$ and
440 $\text{CIT} = 1050$ K, confirming this as the most efficient combustion scenario.

441 As the equivalence ratio increases to stoichiometric ($\phi_{overall} = 1.0$) and
442 rich ($\phi_{overall} = 1.2$) conditions, there is a marked increase in unburned H_2
443 and NH_3 concentrations. For instance, at $\phi_{overall} = 1.2$, the outlet H_2 con-
444 centration reaches over 0.3 vol% at low CIT and remains significantly higher
445 than the leaner cases even as temperature increases. Similarly, NH_3 levels are
446 the highest at $\phi_{overall} = 1.2$, peaking above 3700 ppm at low CIT and gradu-

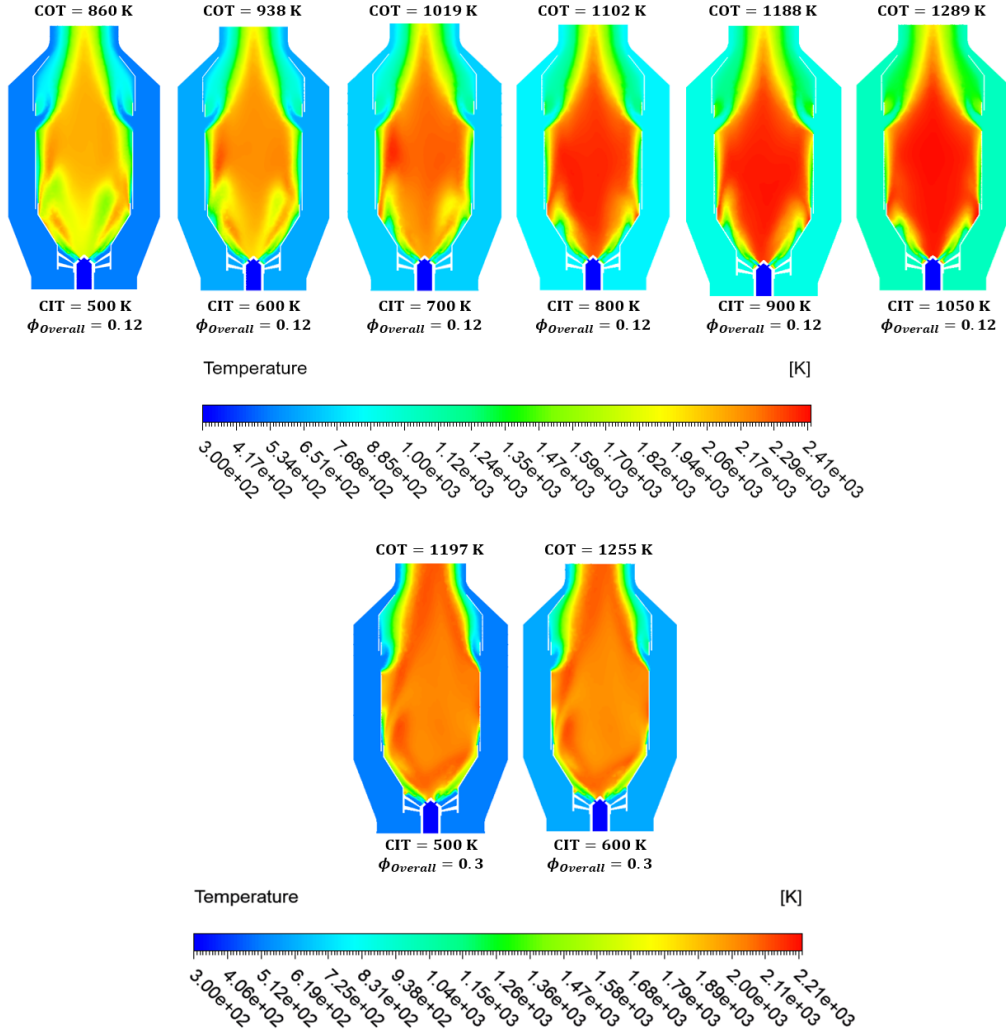


Figure 6: Temperature distribution for different CIT and $\phi_{overalls}$

447 ally declining with increasing temperature. These trends indicate that richer
 448 mixtures result in incomplete combustion and poorer fuel utilization, espe-
 449 cially at lower CITs. While increasing CIT helps mitigate this inefficiency by
 450 enhancing the oxidation of intermediate species, rich conditions still exhibit
 451 substantially higher emissions of unburned fuel components. The results em-
 452 phasize that while higher equivalence ratios produce greater unburned fuel
 453 emissions, increasing CIT remains an effective strategy for improving com-
 454 bustion efficiency. The optimal condition, combining minimal unburned NH_3
 455 and H_2 emissions, remains $\phi_{overall} = 0.12$ at $\text{CIT} = 1050$ K. Importantly, such
 456 lean operation is not unusual: micro gas turbines are typically designed to
 457 run at global equivalence ratios between 0.1 and 0.2 to ensure low NO_x emis-
 458 sions, limit turbine inlet temperature, and preserve component durability
 459 [56, 57].

460 Figure 8a illustrates the variation of outlet dry NO_x emissions, expressed
 461 as concentrations in ppm corrected to 15% O_2 , as a function of the combustor
 462 inlet temperature (CIT) for four overall equivalence ratios: 0.12, 0.3, 1.0,
 463 and 1.2. As expected, NO_x emissions increase with rising CIT, reflecting the
 464 temperature sensitivity of NO_x formation mechanisms.

465 At lower CIT (around 500–600 K), the NO_x emissions for all equivalence
 466 ratios are relatively close, indicating a predominant contribution from fuel-
 467 bound NO_x . However, as CIT increases, clear divergence emerges among
 468 the curves. The leanest mixture ($\phi_{overall} = 0.12$) exhibits the highest NO_x
 469 levels, followed by $\phi_{overall} = 0.3$, while the richer cases ($\phi_{overall} = 1.0$ and 1.2)

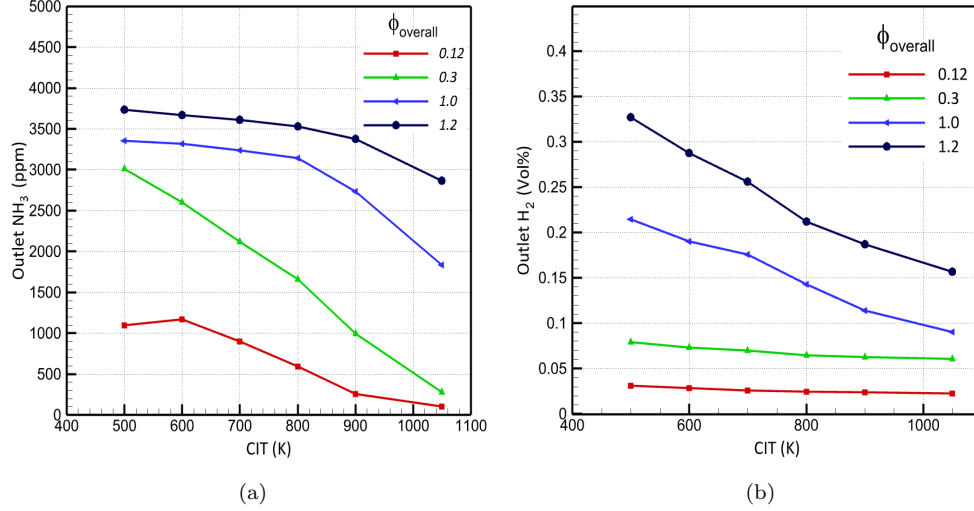


Figure 7: Concentration of (a) ammonia and (b) hydrogen in the outlet of the combustion chamber for different CITs and $\phi_{overall}$ s

display significantly lower emissions across the entire temperature range.

mixtures,

This trend is closely linked to the availability of oxygen in the dilution zone, as shown in Figure 8b. The O_2 mole fraction steadily decreases with increasing overall equivalence ratio, resulting in a progressively oxygen-deficient environment. At low equivalence ratios, excess oxygen facilitates the oxidation of fuel-bound nitrogen to NO_x , thereby enhancing emissions. In contrast, under fuel-rich conditions (higher $\phi_{overall}$), the reduced O_2 availability suppresses this oxidation process, limiting NO_x formation despite increasing CIT.

In the primary combustion zone, significant ammonia cracking takes place, generating a high concentration of nitrogen-containing species such as N_2 and

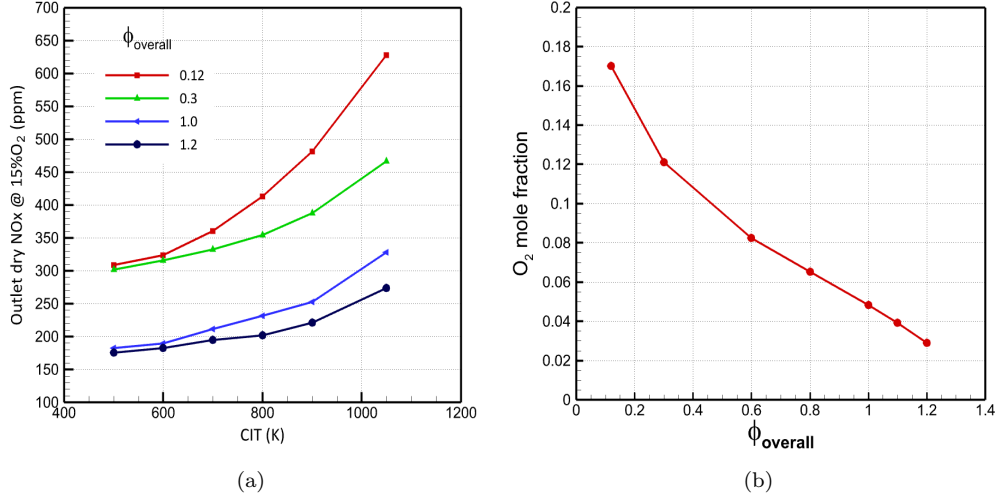


Figure 8: Concentration of (a) Concentration of NO_x emission in the outlet of the combustion chamber for different CITs and $\phi_{overall}$ s (b) Average concentration of O₂ in the dilution zone for different $\phi_{overall}$ s

reactive nitrogen radicals (N). However, despite the abundance of these intermediates, their conversion to NO and NO₂ in the downstream region is suppressed by oxygen deficiency at higher $\phi_{overall}$ values. A more detailed kinetic interpretation, therefore, confirms that fuel-NO is the dominant formation pathway across all studied conditions. At high combustor inlet temperatures (CIT > 900 K), thermal NO via the extended Zeldovich mechanism becomes increasingly relevant, but its contribution remains secondary compared to fuel-NO. Prompt NO, which requires hydrocarbon-derived CH radicals, is negligible in the present case since the Stagni mechanism [52] does not include C-containing species.

For a range of overall equivalency ratios, Figure 9 shows the combustor output power at different CITs. The efficiency for the leanest scenario

494 ($\phi_{overall} = 0.12$) is shown by the column bars. It is clear from the figure that
 495 all $\phi_{overall}$ s experience an increase in output power as the CIT rises. The
 496 output power is maximum under the conditions with $\phi_{overall} = 0.12$ and CIT
 497 = 1050 K. Higher input temperatures improve reaction rates and combustion
 498 efficiency, which increases power generation. From the efficiency point of
 499 view, the lean scenario ($\phi_{overall} = 0.12$) exhibits a notable improvement as the
 500 CIT increases. Efficiency is relatively low at 500 K but grows dramatically
 501 as the CIT rises, peaking at 1050 K. The efficiency rises from CIT = 500 K
 502 to CIT = 1050 K by almost 85%. This demonstrates how temperature significantly
 503 impacts combustion performance, especially under lean conditions
 504 where response rates are more sensitive to temperature. The efficiency values
 505 were calculated based on the ratio of output power to the nominal power of
 506 20 kW. As a result, the increase in efficiency reflects the system's ability to
 507 convert the available energy more effectively at higher temperatures. However,
 508 while higher CIT improves efficiency and power output, it may also
 509 impact NO_x emissions, which should be considered in practical applications.

510 Figure 10 illustrates the effect of air inlet temperature on the heat release
 511 rate iso-surface, colored by the ammonia mole fraction, in the combustion
 512 chamber with the overall equivalence ratio of 0.12. The iso-surface is defined
 513 at a heat release rate of $3 \times 10^9 \text{ W/m}^3$, which corresponds to 5% of the maximum
 514 heat release rate. This threshold was selected to capture the primary
 515 reaction zones effectively while filtering out minor heat release fluctuations
 516 that could obscure the overall flame structure. At a lower inlet temperature

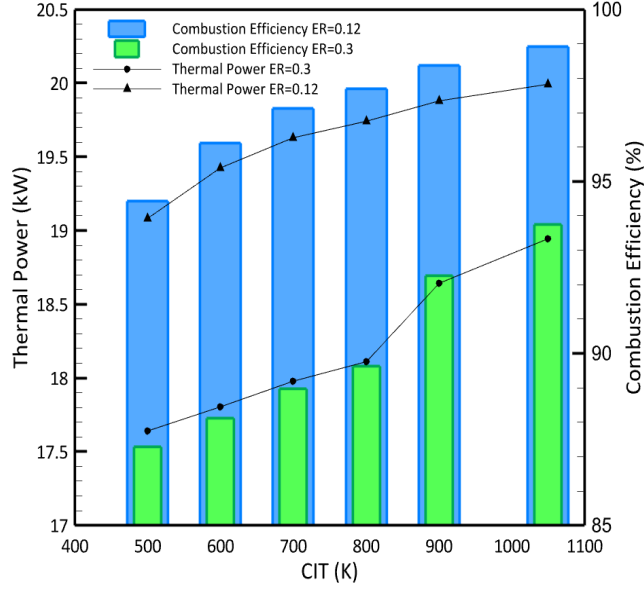


Figure 9: Combustor output power and efficiency at different combustor inlet temperatures (CITs) for various $\phi_{overall}$ s.

517 of 500 K, the heat release region remains more localized near the injector,
 518 with a higher ammonia mole fraction in the reaction zone, indicating in-
 519 complete combustion and lower reaction efficiency. In contrast, at CIT =
 520 1050 K, the heat release zone extends further downstream, and the ammonia
 521 mole fraction decreases in the reaction region, suggesting improved oxidation
 522 and enhanced combustion efficiency. The higher inlet temperature promotes
 523 faster chemical reactions, leading to better flame propagation and a more
 524 distributed heat release zone. This improved combustion behavior reduces
 525 ammonia slip, potentially enhancing overall efficiency. However, its impact
 526 on NO_x emissions, as discussed before, is considerable (Figure 8a).

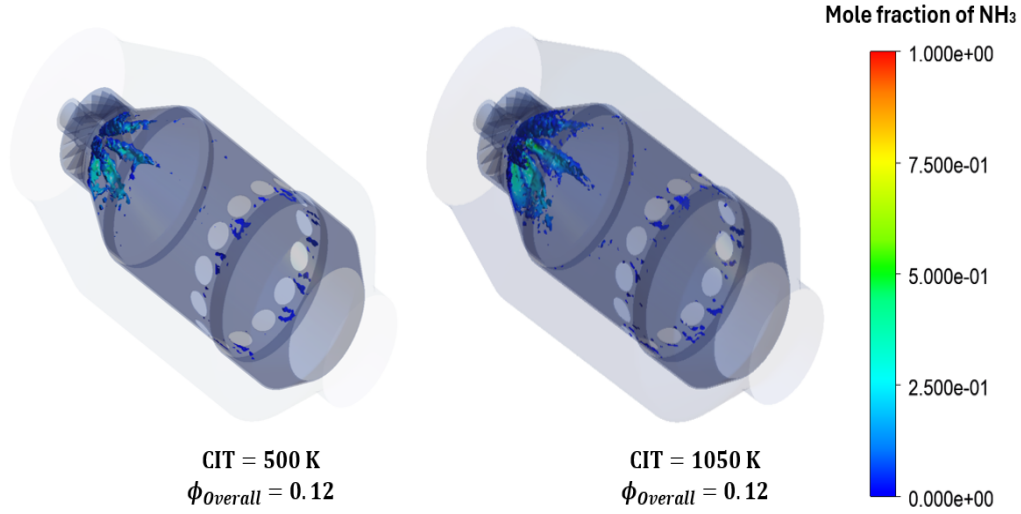


Figure 10: Heat release rate iso-surface at $3 \times 10^9 W/m^3$ (5% of the maximum heat release rate), colored by ammonia mole fraction.

527 4. Conclusion

528 This study investigates the impact of Combustor Inlet Temperature (CIT)
 529 on emissions, performance, and combustion characteristics in an optimized
 530 staged rich-lean, non-premixed ammonia-fueled micro gas turbine combus-
 531 tion chamber through detailed CFD simulations. The findings reveal that
 532 increasing CIT from 500 K to 1050 K at an overall equivalence ratio of 0.12
 533 induces significant changes in combustion behavior, including a 430 K rise in
 534 combustor outlet temperature (COT) and a 5% improvement in combustion
 535 efficiency. Higher CIT also leads to reduced unburned NH₃ and H₂ emissions,
 536 indicating enhanced oxidation and fuel utilization. However, the results show
 537 a substantial increase in NO_x emissions with rising CIT.

538 Although higher overall equivalence ratios were studied, values above 0.3

were found to be impractical due to excessive combustor outlet temperatures, increased NO_x emissions, and incomplete combustion under certain conditions. The analysis highlights that very lean conditions ($\phi \approx 0.12$) provide the lowest emissions and most stable flame structure, but at the expense of thermal efficiency. At moderately lean conditions ($\phi \approx 0.3$), combustion efficiency improves, yet the outlet temperature approaches turbine material limits, and NO_x emissions increase significantly, particularly at elevated CIT. These results demonstrate the sensitivity of turbine performance to equivalence ratio, with a clear trade-off between efficiency, NO_x emissions, and flame stability. Overall, the findings confirm that elevated CIT enhances combustion and thermodynamic efficiency in mGTs, but effective operation requires a balance between lean stability and efficiency, supported by advanced NO_x mitigation strategies beyond staged rich-lean approaches, such as post-treatment systems.

This study highlights some practical implications in the use of ammonia for micro-gas turbine combustors:

- Designers of ammonia-fueled micro gas turbines should optimize for elevated CIT to enhance efficiency.
- Maintaining an overall equivalence ratio near 0.12 balances emissions and performance.
- NO_x emissions must be controlled through advanced mitiga-

560 **tion technologies alongside combustion optimization.**

561 Overall, this study provides valuable insights toward optimizing ammonia-
562 based micro gas turbines, advancing carbon-free power generation. Future
563 work should integrate additional NO_x reduction techniques and experimen-
564 tal validation to refine sustainable combustion strategies for ammonia energy
565 systems.

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