

Full Length Article

The influence of radiation modeling on flame characteristics and emissions prediction in microcombustors with Ammonia/Hydrogen blends

De Giorgi Maria Grazia^{a,*}, Cinieri Giacomo^a, Marseglia Guido^a

^a University of Salento, Department of Engineering for Innovation, Via per Monteroni, 73100 Lecce, Italy

ARTICLE INFO

Keywords:

Hydrogen

Ammonia

Absorption coefficient

Radiation

Green fuels

ABSTRACT

This study advances numerical methodologies for designing microcombustor-based thermophotovoltaic systems by incorporating comprehensive analyses of radiation models and absorption coefficients. It examines the impact of non-premixed hydrogen-ammonia-air fuel blends on the micro combustion process using three-dimensional CFD simulations on a Y-shaped microcombustor under atmospheric conditions.

Key to this research is modeling radiative heat transfer from multiple species, including ammonia (NH₃), nitric oxide (NO), and water vapor, ensuring accurate predictions and optimization of thermal behavior and efficiency. Three modeling approaches were compared: a multispecies Planck-mean approximation radiation model (PMAC), a narrowband model for water vapor, and a scenario excluding radiation effects.

The PMAC model, incorporating the absorption coefficients of ammonia and its products, consistently produced lower errors in flame length compared to the NB method across all equivalence ratios, with errors ranging from 0 % to 7 % for PMAC and 10 % to 30 % for NB, with the lowest error observed at $\Phi = 1.0$. Additionally, the prediction of laminar burning velocity (LBV) differed by approximately 4 % between the two models.

Considering different fuel blends, two scenarios were compared: constant input thermal power and constant fuel flow rate. Efficiency in the constant input thermal power scenario maintained higher radiation efficiency, in the range of 32–38%. Additionally, radiation efficiency initially increased with increasing H₂ content but subsequently decreased for high H₂ values due to effects on flame area, flame position, and temperature.

1. Introduction

Recent advancements in combustion-based microdevices have been propelled by the advantageous properties of hydrocarbons, such as their high energy density, reduced weight, and compact dimensions [1–7]. Microcombustors are crucial in modern energy solutions, delivering efficient power in compact packages. Ideal for portable power generators and miniature propulsion systems, they convert fuel into energy within a small footprint. This efficiency enhances portability, reduces material use, and simplifies system architecture. Their compactness and high energy output make microcombustors indispensable for advancing sustainable and efficient energy technologies, essential for sectors relying on reliable and lightweight autonomous power sources.

Maintaining a stable flame in microcombustors presents significant challenges due to their high area-to-volume ratios and short mixture residence times [8,9]. These factors complicate achieving controlled, efficient combustion, as the compact size of the combustion chamber often leads to rapid heat losses and quenching effects. Such conditions

cool the flame too swiftly, potentially leading to flame extinction. Additionally, the brief residence time available in these systems may prevent chemical reactions from completing, resulting in unstable combustion and variable thermal outputs. A well-conceived microcombustor design hinges on a deep understanding of chemical reaction dynamics and heat transfer processes. Detailed analysis is essential to determine the optimal geometrical configuration and materials that can withstand high temperatures and corrosive environments while enhancing combustion efficiency [10,11]. Li et al. [12] developed a symmetrical catalytic micro-combustor with methane/air mixture aimed at achieving stable combustion. Their findings indicated that the inlet velocity could exceed 9 m/s, with maximum combustion and surface radiation efficiencies reaching 98.5 % and 25.9 %, respectively. They also discovered that enhancing the wall thermal conductivity could increase both wall temperature and radiant energy output, thereby boosting energy conversion efficiency. Optimizing microcombustor configuration is also crucial for minimizing emissions of carbon products and nitrogen oxides (NO_x) [13–16]. In particular for ammonia application, Tang et al. [14] introduced a baffle structure and

* Corresponding author at: Department of Engineering for Innovation, Via per Monteroni, 73100 Lecce, Italy.

E-mail address: mariagrazia.degiorgi@unisalento.it (D. Giorgi Maria Grazia).

<https://doi.org/10.1016/j.fuel.2024.132759>

Received 25 April 2024; Received in revised form 26 July 2024; Accepted 8 August 2024

Available online 14 August 2024

0016-2361/© 2025 The Authors. Published by Elsevier Ltd. This is an open access article under the CC BY license (<http://creativecommons.org/licenses/by/4.0/>).

Nomenclature		PMAC	Planck Mean Absorption Coefficient
$A_{we,i}$	External wall cell Area of mesh face i	T_0	Ambient temperature, 300 K
d	Wall thickness (m)	T_{exit}	Outlet mean temperature (K)
GCI	Grid Convergence Index	T_{fmax}	Max Flame temperature (K)
h_0	Heat transfer coefficient (W/Km ²)	T_{wi}	Internal wall temperature (K)
H_2	Hydrogen	T_{we}	External wall temperature (K)
HITRAN	High-Resolution Transmission Molecular Absorption Database	v_{air}	Velocity of air (m/s)
LBV	Laminar Burning Velocity (m/s)	v_{fuel}	Velocity of fuel (m/s)
L_f	Flame length (m)	WSSGM	Weighted-sum-of-gray-gases model
LHV	Lower Heating Value (MJ/kg)	x_{H2}	Fuel hydrogen molar fraction
MTPV	Microthermophotovoltaic System	<i>Greek Letters</i>	
$\dot{m}_{fuel}$	Fuel mass flow rate (kg/s)	α	Absorption coefficient (1/m)
NB	Narrow Band	ε	Quartz glass absorption coefficient, 0.93
NH_3	Ammonia	ε_f	Hydrogen power fuel fraction
NO_{exit}	Outlet mean mole fraction	η	Radiation Efficiency (%)
NO_x	Nitrogen oxides	η_c	Combustion efficiency
O_{max}	Max NO molar fraction	σ	Boltzmann constant
P	Pressure, 1 atm	ρ	Density (kg/m ³)
P_R	Emitted radiant power	Φ	Equivalence ratio
P_H	Fuel input power (W)	λ	Thermal conductivity (W/mK)

a secondary fuel injection strategy enhancing flame stability and wall temperature while reducing NO emissions by improving the reaction between NO and ammonia and increasing the average wall temperature by 5.2 % compared to conventional designs. Although increasing the secondary fuel injection ratio significantly reduces NO emissions, it also increases ammonia leakage.

The past few decades have seen a significant pivot towards cleaner combustion technologies, emphasizing the development and utilization of carbon-free fuels such as hydrogen (H_2) and ammonia (NH_3) to achieve cleaner combustion and mitigate emissions [17,18]. Hydrogen, known for its high energy yield per unit mass and zero carbon emissions upon combustion, has emerged as a leading option. Ammonia, while not yielding energy as high as conventional hydrocarbons, presents a viable carbon-free alternative due to its substantial hydrogen content and ease of liquid storage. Ammonia intrinsic properties, such as its lower flame propagation speed and chemical reactivity compared to hydrocarbons, necessitate rigorous combustion conditions, especially within the confines of microcombustors [19]. Its high minimum ignition energy, relatively low calorific value, and narrow flammability range make ammonia a challenging fuel to burn efficiently on its own. Consequently, it is frequently blended with other fuels that can enhance its combustion, such as hydrogen, which can significantly improve the flame speed and extend the flammability limits [20–22]. Blending ammonia with methane (CH_4) has already demonstrated its capability to reduce carbon emissions, offering a viable path to decrease the carbon footprint of energy systems [23–25]. Zheng et al. [20] conducted a numerical study on blended CH_4/NH_3 premixed flames at different equivalence ratios. Their results indicated that the improvement in flame speed due to radiation exhibited a nonlinear trend as the equivalence ratio increased. For equivalence ratios between 0.6 and 1.2, preheat-induced chemical effects were dominant, while for ratios between 1.2 and 1.5, direct radiation effects took precedence. Additionally, the effect of radiation reabsorption on NO formation initially decreased and then increased with higher equivalence ratios, controlled by the reactions $NH+NO \rightleftharpoons N_2O+H$ and $NH+O_2 \rightleftharpoons NO+OH$ in lean combustion, and $N+OH \rightleftharpoons NO+H$ and $NH+O \rightleftharpoons NO+H$ in rich combustion.

The challenge of NOx emissions remains prominent, especially in NH_3 /air-premixed flames, where high combustion temperatures can lead to significant NOx production [26].

Blending NH_3 with hydrogen is an effective strategy to minimize

emissions. Integrating ammonia (NH_3) and hydrogen (H_2) in combustion systems reduces the environmental footprint of energy technologies. This approach combines ammonia's carbon-free attribute with hydrogen's high combustion efficiency, significantly lowering harmful emissions. Hydrogen enhances the burn rate and expands the flammability limits of ammonia, leading to more complete combustion and reduced NOx emissions compared to burning ammonia under fuel-lean conditions. [27–29]. Luo et al. [29] studied the premixed combustion of $NH_3/H_2/O_2$ in a segmented nozzle MTPV micro-combustor. Their findings revealed that the mean wall temperature of the segmented micro-combustor was 11.5 K higher than that of a non-segmented micro-combustor, and NO emissions were reduced by up to 7.91 %. When the mass fraction of hydrogen in the gas mixture increased from 10 % to 30 %, radiation efficiency improved by 13.5 %, but NO emissions also increased. To mitigate NO emissions, fuel-rich combustion was considered. In fact, rich mixtures typically result in better combustion efficiencies and lower NOx emissions when using ammonia-hydrogen blends [30].

This enhanced understanding of ammonia and hydrogen use in combustion systems, alongside strategies for reducing NOx emissions, is further complemented by emerging research that emphasizes the integration of thermophotovoltaic and thermoelectric systems in ammonia-hydrogen energy devices.

Research, such as the work by Zhang et al. [31], evaluates the nuances of fuel inlet configurations and flame dynamics within a two-stage thermophotovoltaic-thermoelectric energy conversion system, specifically analyzing an ammonia-oxygen mixture. Their findings underscore the critical balance between maintaining optimal outer wall temperatures and maximizing energy conversion efficiency while managing NO emissions [31]. Similarly, You et al. [32] explore the effects of flow rates and mixture compositions in H_2 -air mixtures, revealing that efficiency peaks at stoichiometric conditions before diminishing in richer mixtures. These studies highlight the delicate interplay between combustion parameters and system performance, illustrating the importance of precise control over these variables.

The role of radiation in the modeling of combustion of these fuels should not be underestimated, as ignoring its impact can lead to significant discrepancies in NO concentration estimates and overall system efficiency, particularly in fuel blends with hydrogen [33]. Comprehensive reviews and comparisons of radiation models, such as those

conducted by Mazumder and Roy [34], Lawi and Majhool [35], and Caetano et al. [36], stress the necessity for detailed and accurate modeling approaches. These models are essential for predicting thermal radiation heat loss, influencing flame behavior and heat flux in both gas and combustion wall interactions, as explored by Razmjooei et al. [37]. Additionally, Yang et al.'s proposal for a new methodology to estimate flame radiation in environments with suspended particles [38] points to the ongoing evolution of this field, suggesting that understanding and integrating radiation effects are pivotal for advancing combustion technology. Their results revealed that for a typical lab-scale air-fired flame, wall emissions and reflections could account for up to 55 % of the measured incident radiation for a refractory-lined wall and 40 % for a water-cooled wall. In the context of microcombustion, radiation losses and reabsorption significantly impact heat transfer dynamics. This contrasts with traditional combustion studies that tend to downplay radiation effects due to the small scale of reaction involved [39]. Recent research has broadened the focus on radiation effects in combustion, emphasizing not only the radiative heat loss and reabsorption of reagents and products but also exploring the influential role of radicals and fuels themselves. Historically, the study of radiation in combustion has leveraged databases like the High-Resolution Transmission Molecular Absorption Database (HITRAN), traditionally used in fields ranging from astronomy to meteorology. For instance, Grigor'ev et al. [40] utilized HITRAN and ACE-FTS data to enhance models of Earth atmospheric brightness and transmission by improving air absorption coefficients under varied environmental conditions. Similarly, Li et al. [41] demonstrated the utility of HITRAN in developing techniques for measuring atmospheric oxygen density using stellar occultation methods.

The HITRAN database, however, has certain limitations, particularly in its coverage of the ultraviolet (UV) spectrum, which restricts its application in areas such as aerospace optics and optical detection. Addressing this, Du et al. [42] have proposed expanding the database to encompass a broader UV spectrum, thereby enhancing its utility for more diverse applications. Despite these challenges, the database has significantly advanced the study of clean fuel combustion, particularly through its detailed spectral data which allows for more accurate modeling of thermal radiation effects in combustion processes.

Moreover, studies have shown that incorporating radiation reabsorption models can markedly increase planar and spherical laminar flame speed forecasting, as seen in methane, ammonia, and hydrogen/air flames, where radiation models have outperformed traditional adiabatic approaches [20,43]. The significance of accurate radiation models is exemplified by Liu et al. [44], who showed that radiation reabsorption in syngas flames with CO₂ and H₂O at higher pressures significantly affects laminar flame speeds. The PMAC approach in this study, using HITRAN data, provides a comprehensive evaluation of how different gas species impact radiation within the combustion chamber [45]. This is crucial in systems where ammonia and hydrogen play dominant roles, such as ammonia combustion where gases other than water vapor significantly influence heat transfer [46]. The PMAC method considers key species in hydrogen/ammonia combustion: hydrogen (H₂), ammonia (NH₃), oxygen (O₂), nitrogen (N₂), hydroxyl (OH), water vapor (H₂O), nitric oxide (NO), and nitrogen dioxide (NO₂). Each component interacts with radiation differently, affecting the overall energy balance in the combustion chamber.

Detailed radiation modeling is crucial for optimizing combustion efficiency and emissions and for designing systems that effectively use ammonia and hydrogen as sustainable fuels. This aligns with broader objectives of reducing emissions and improving energy conversion efficiency in clean fuel technologies, underscoring the importance of advanced radiation models in modern combustion studies [46].

Building on the groundwork laid by the detailed spectral analysis provided by the PMAC method, this research introduces a meticulous comparison of radiation absorption effects using a narrow-band water vapor absorption coefficients model across multiple spectral bands and a

novel approach by integrating HITRAN absorption coefficients within a three-dimensional computational fluid dynamics (CFD) analysis. Only two studies have investigated ammonia/hydrogen/air mixtures for MTPV systems, and both were conducted under premixed conditions [47,48]. Mohammadpour et al. [3] conducted an analysis with varying inlet velocities and air dilution levels with N₂. The results indicate that increasing inlet velocity within the studied range enhances the uniformity of temperature distribution in both the fluid and solid domains. The maximum total energy conversion efficiency achieved was 8.2 %, corresponding to an output electric power of 6.6 W. However, higher air dilution levels (up to 84 % N₂ by volume) significantly improve temperature distribution uniformity, leading to a decrease in mean temperature and overall thermo-photovoltaic efficiency. Han et al. [47] performed a comparative analysis of flame stability behaviors between hydrogen/ammonia/air blended combustion in both conventional and proposed wavy combustors revealing a broadened blowout limit in the wavy designs. The study found that the wavy micro-combustor could achieve approximately a 21.2 % reduction in NO_x emissions. The NO_x emission reduction improved progressively with an increase in the nitrogen fuel mass ratio.

For the first time, the present study analyzed a non-premixed H₂-NH₃-air analysis in a Y-shaped MTPV system. Moreover, this research assesses the impact of varying concentrations of hydrogen and ammonia in air on the operational efficiency of a microthermophotovoltaic system and its emissions profile, maintaining a constant mass flow rate input power. The influence of different equivalence ratios is also analyzed, providing a view of the interaction between fuel composition and combustion efficiency. This multifaceted analysis advances the understanding of ammonia and hydrogen as sustainable fuels, highlighting the critical role of precise radiation modeling in enhancing the performance and environmental sustainability of energy systems.

2. Methodology

2.1. Mathematical models

The computational fluid dynamics (CFD) simulations are carried out using ANSYS Fluent 23.0 [49] to solve the governing fluid equations in a Y-shaped microcombustor fueled by a blend of hydrogen and ammonia. The key equations considered include those for conservation of mass, momentum, heat transfer, and chemical species (Equations (1)–(5)):

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0 \quad (1)$$

$$\frac{\partial(\rho u_j)}{\partial t} + \frac{\partial(\rho u_i u_j - \tau_{ij})}{\partial x_i} = \frac{\partial p}{\partial x_j} \quad (2)$$

$$\frac{\partial(\rho h)}{\partial t} + \frac{\partial(\rho u_i h)}{\partial x_i} = \frac{\partial(\lambda \partial T_f)}{\partial t} - \sum_j^n \frac{\partial(h_j J_j)}{\partial x_i} + \sum_j^n h_j R_j \quad (3)$$

$$\frac{\partial(\rho Y_i)}{\partial t} + \frac{\partial(\rho u_i Y_i)}{\partial x_i} = \frac{\partial J_i}{\partial x_i} - R_i \quad (4)$$

$$Q_{\text{loss}} = h_0 A (T_{\text{we}} - T_0) + \varepsilon \sigma A (T_{\text{we}}^4 - T_0^4) \quad (5)$$

In this context, we define ρ as the gas density, p as the pressure, and u as the velocity. The stress tensor is represented by τ_{ij} , while h denotes the total enthalpy. The diffusion flux of a species i is given by J_i , with Y_i representing its mass fraction. The temperature is denoted by T , and R_j is the net rate of production of species j due to chemical reactions. The parameter i refers to the species index, d the wall thickness and λ represents thermal conductivity. The model also incorporates an ideal gas flow model and a mixing law for the specific heat capacity, C_p . The effects of convection and radiation are considered in computing heat losses, using for radiation the Radiative Transfer Equation (RTE) and the

DO ALGORITHM with the Finite Angle Method (FAM) to discretize the solid angle and ensure energy conservation. In the solid region the following energy equation is included:

$$\frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T_w}{\partial x_i} \right) = 0 \quad (6)$$

Different modeling approaches for the spectral absorption coefficient are considered, as described in the next section.

2.2. Absorption coefficient modelling

One of the key aspects in radiative analysis is the value of the mixture absorption coefficient which is an essential input parameter in radiative transfer equation computations. Its estimation is a crucial element in the study of combustion and radiation impact. Several methods exist in the literature to estimate this parameter. Quantum mechanics dictates that energy levels are discrete or quantized, meaning only photons with specific energy or frequency can be absorbed. Similarly, photons of certain frequencies are emitted during transitions from higher to lower energy levels. As a result, the absorption and emission spectra of most molecular gases display a pronounced line structure that may be aggregated into bands. Over the last decades, the position and intensity of these spectral lines have been documented in the HITRAN database. Wide-band models simplify this process by averaging the properties over a band rather than calculating them at each wavenumber. This approach is particularly useful for gases with dense line spectra that would be computationally intensive. The grey gas approach assumes that each cell contains a gray gas, a term referring to a gas with constant properties across all wavelengths. Mixture components occupy a portion of the cell, and the occupied value is determined by the number of moles according to Amagat's law. The involved equation is [50]:

$$\alpha = \sum_i^n \alpha_i = \sum_i^n S_i F(\eta - \eta_i) \quad (7)$$

α_i the absorption coefficient of spectral line i , S_i the spectral integral intensity, $F(\eta - \eta_i)$ absorption spectral line shape. More methodology details are provided in [50]. Computations were conducted for species temperature between 300 and 1500 K, 100 K step. To express these coefficients, a fitting tool is employed to establish a polynomial function for relevant chemical species in ammonia/hydrogen combustion and then they are expressed in the final absorption coefficient formula. NB model doesn't assume gray gases and divides the spectrum into narrower segments, allowing for a more accurate representation of the spectral properties of the gas when higher accuracy is required balancing computational efficiency with spectral accuracy. For our purposes, it was applied to H₂O. The two approaches will be compared

and the effects analyzed in 3-D CFD microcombustor analysis. Absorption coefficients have been estimated using RADIS, an open-source code for nonequilibrium emission and absorption infrared line-by-line analysis [51]. This tool is developed with a focus on molecules in their electronic ground state, utilizing databases like HITRAN, HITEMP, and CDS. The tool includes a line survey feature, a built-in look-up database to expedite convergence times during experimental spectra fitting, and a multi-slab module for simulating line-of-sight experiments. The spectral emissivity is obtained from the spectral transmittance using Kirchhoff law and multiplying it by the Planck function results in the spectral radiance. Fig. 1a and b depict the spectral absorption coefficients for NH₃ and H₂O calculated by RADIS at low x_{H_2} conditions test cases (see chapter 3.1 and supplementary materials for flame temperature and species concentrations).

Distinct absorption bands are visible in specific wavelength intervals, with significant peaks around 1500 nm, 2000 nm, and over 3000 nm having low absorbance outside of the peak bands. The scale of the ordinate axis shows the absorption coefficient, which reaches a maximum value greater than 5 cm⁻¹ indicating regions of strong absorption. In Fig. 2a, the PMAC model illustrates the variation of α for various species over the temperature range. The graph reveals a stark decrease in the absorption coefficient for NO as temperature rises. NH₃ and H₂O both demonstrate a decrease in their absorption coefficients after peaking between 700 K and 800 K. Beyond these temperatures, the curves level off, suggesting that their absorption properties are less sensitive to temperature changes in this range. The application of the grey gas model in this context simplifies the spectral characteristics of the gases. It averages their absorptive properties across the infrared spectrum and emphasizes the effects of temperature, instead of providing a detailed account of the spectral lines for each gas. This approach, while less precise spectrally, can often be useful in understanding the broader temperature-dependent behavior of gas absorption in these species. In Fig. 2b, the temperature-dependent behavior of H₂O vapor absorption coefficients across several spectral bands within the NB model has been shown. The plot illustrates how absorption varies with temperature for each band, detailing the water vapor α from the near-infrared (NIR) to the mid-infrared spectral region. The absorption coefficient has been estimated within seven specific spectral bands, with their corresponding wavelength ranges implemented in the simulation code using User-Defined Functions (UDFs). Band 2, covering the 3 to 4.16 μ m range, shows a marked absorption at cooler temperatures, which decreases substantially with rising temperatures. This trend indicates that water vapor has a significant absorption capacity in the spectral region near the source of infrared radiation at lower temperatures, which diminishes with increasing temperature, due to the effects of Doppler broadening [52]. The phenomenon of α decreasing with

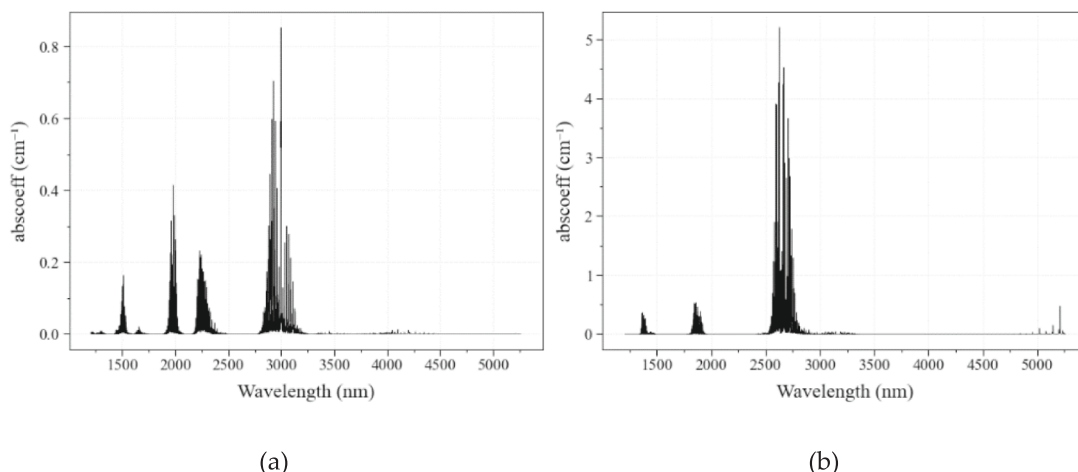


Fig. 1. Spectral absorption coefficient of at 2000 K and 1 atm a) NH₃ mole fraction = 0.2b) H₂O mole fraction = 0.3.

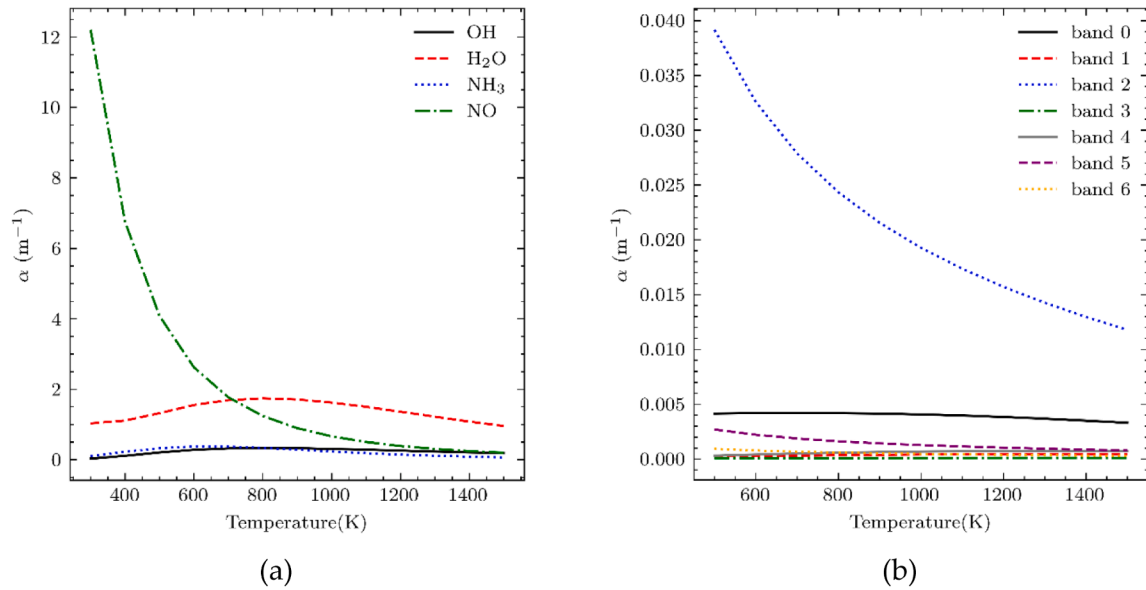


Fig. 2. a) pmac spectral absorption coefficient in the function of temperature and 1 atm; b) NB H₂O Spectral absorption coefficient for H₂O mole fraction = 0.2b) H₂O mole fraction = 0.3.

temperature is attributed to the Doppler broadening effect. This broadening occurs due to the velocity distribution of atoms or molecules involved in emission or absorption processes. With an increase in temperature, there's an increase in the thermal motion of these particles, influencing the frequency of the radiation they emit or absorb. This Doppler effect becomes more significant at elevated temperatures, as the intensified thermal motion leads to a wider velocity distribution, resulting in a broader spectrum of thermal Doppler shifts [52,53]. The absorption in other bands appears to remain relatively constant across the temperature spectrum, suggesting that an average value could be used to approximate the absorption coefficient within these ranges. Notably, bands 0, 2, and 5 stand out for their absorption characteristics, while the other bands have minimal absorption, falling within the so-called water vapor windows, where absorption by water vapor is significantly less impactful. These windows are identified in the literature as regions where the atmospheric transmittance is relatively high due to low absorption by water vapor, allowing radiation to pass through more easily [54,55]. Finally, the α fit functions utilized in the NB and PMAC models are presented in Tables 1 and Table 2.

2.3. Kinetic mechanism

Enhanced kinetic mechanisms for fuel-air mixtures have been adopted. The combustion model, building on the foundational work by Mei et al. [56], incorporates the hydrogen mechanism developed by Hashemi et al. [57] and integrates the ammonia sub-mechanism from Shrestha et al. and Konnov [58,59]. This comprehensive mechanism includes a total of 287 reactions and 39 species. Validation was conducted using the Cantera software, where the predicted Laminar

Table 1
NB model absorption coefficients.

Band	Start-end λ (μm)	α (m ⁻¹)
0	0–2.2	0.00392
1	2.22–3.22	0.00038
2	3.22–4.16	$-3\text{E-}11 \text{ T}^3 + 1\text{E-}7 \text{ T}^2 + 0.0002 \text{ T} + 0.0923$
3	4.16–4.65	8.61E-05
4	4.65–5.12	0.000605
5	5.12–6.25	0.0014
6	6.25–10	0.0005

Table 2
PMAC model absorption coefficients.

Species	α (m ⁻¹)
OH	$6.0623\text{e-}10 \cdot \text{pow}(\text{T}, 3) - 2.2631\text{e-}06 \cdot \text{pow}(\text{T}, 2) + 2.523\text{e-}03 \cdot \text{T} - 5.568\text{e-}01$
H ₂ O	$3.836\text{e-}12 \cdot \text{pow}(\text{T}, 4) - 1.291\text{e-}08 \cdot \text{pow}(\text{T}, 3) + 1.279\text{e-}05 \cdot \text{pow}(\text{T}, 2) - 3.185\text{e-}03 \cdot \text{T} + 1.118\text{e} + 00$
NH ₃	$-6.712\text{e-}13 \cdot \text{pow}(\text{T}, 4) + 3.724\text{e-}09 \cdot \text{pow}(\text{T}, 3) - 7.137\text{e-}06 \cdot \text{pow}(\text{T}, 2) + 5.269\text{e-}03 \cdot \text{T} - 9.464\text{e-}01$
NO	$3.465\text{e-}11 \cdot \text{pow}(\text{T}, 4) - 1.481\text{e-}07 \cdot \text{pow}(\text{T}, 3) + 2.335\text{e-}04 \cdot \text{pow}(\text{T}, 2) - 1.627\text{e-}01 \cdot \text{T} + 4.346\text{e} + 01$

Burning Velocity (LBV) was compared against experimental data, as depicted in Fig. 3. This validation process accounted for the radiation absorption coefficient and radiation heat losses in the Cantera free flame model. For reliable solution convergence, the GRAD and CURVE parameters were adjusted to 0.005, across more than 500 grid points. Fig. 3a and 3b illustrate the LBV outcomes, comparing the NB and PMAC models with experimental results, across different hydrogen mole fractions (x_{H_2}) and inlet temperatures for an equivalence ratio (Φ) of 1 [60,61]. Fig. 3a specifically details the influence of varying hydrogen mole fractions (x_{H_2}) on LBV outcomes, whereas Fig. 3b focuses on how changes in inlet temperatures impact LBV for pure ammonia. At inlet temperatures below 350 K, the disparities in LBV results among the radiation models remain below 1 %. In contrast, at higher temperatures, the LBV data from the NB model exhibit increases of 3–4 % over those from the PMAC model, as shown in Fig. 3b. Notably, the differences between the models become negligible when x_{H_2} exceeds 0.4.

2.4. Test case

A standard micro TPV device consisting of three primary elements: a micro combustor/emitter, a filter, and photovoltaic cells. In the device, fuel's chemical energy is transformed into thermal energy in the micro combustor, which raises the temperature of the combustor wall enough to emit numerous photons. These photons then pass through a filter, which serves a dual role. It reflects photons with energy below the bandgap energy of the photovoltaic cells back to the micro combustor for reuse, while allowing photons with higher energy levels to pass through and reach the photovoltaic cells. Once there, these photons

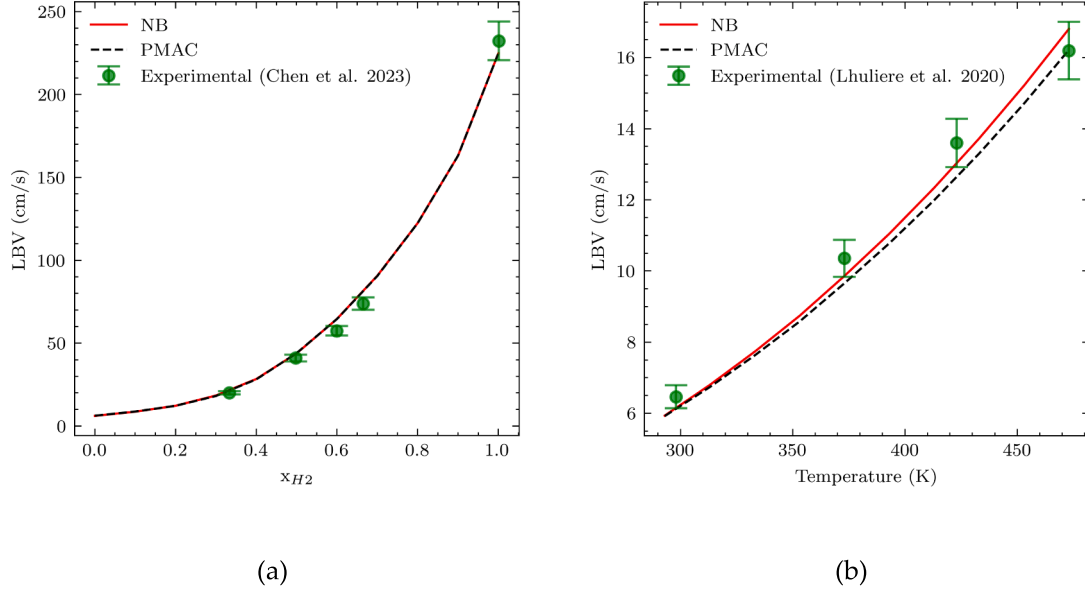


Fig. 3. LBV Validation at 1 atm: a) NB and PMAC models at $T=298$ K, $\Phi = 1$, varying x_{H_2} . b) NB and PMAC models at $\Phi = 1$, varying T with $x_{H_2} = 0$.

generate free electrons, resulting in the production of electrical power. Consequently, the thermal efficiency of the micro combustor is key to enhancing the overall performance of micro-TPV power generators.

This study examines a 3D model of a Y-shaped combustion chamber, characterized by a 200 mm length and cross-sectional area of 2 mm x 1.57 mm with a 90-degree bifurcation. It features dual inlet channels, one for blended fuels and the other for dry air (velocity = 5.29 m/s) maintained at 300 K. Detailed geometry specifics and experimental validations are extensively documented by Xiang et al. [62,63]. In micro thermophotovoltaic (MTPV) devices, the Y-shaped design is pivotal in finely adjusting flow rates and mixture compositions and was previously studied by us with plasma and ammonia [64–66]. The chamber is

constructed from quartz glass with an emissivity (ϵ) of 0.93 and operates under standard conditions of 1 atm and 300 K.

To enhance computational efficiency, a symmetry plane boundary condition is applied to half of the model. The simulation adopts a three-dimensional steady-state approach, disregarding the effects of gravity, and employs a second-order scheme. A coupled algorithm manages the pressure–velocity coupling, ensuring a robust computational framework. Convergence is confirmed when residuals for all parameters drop below

10^{-3} , with particular attention to the convergence of H_2O , OH , and temperature within the reaction zone. The wall of the combustion chamber is treated as a no-slip wall, optimizing the fidelity of the flow

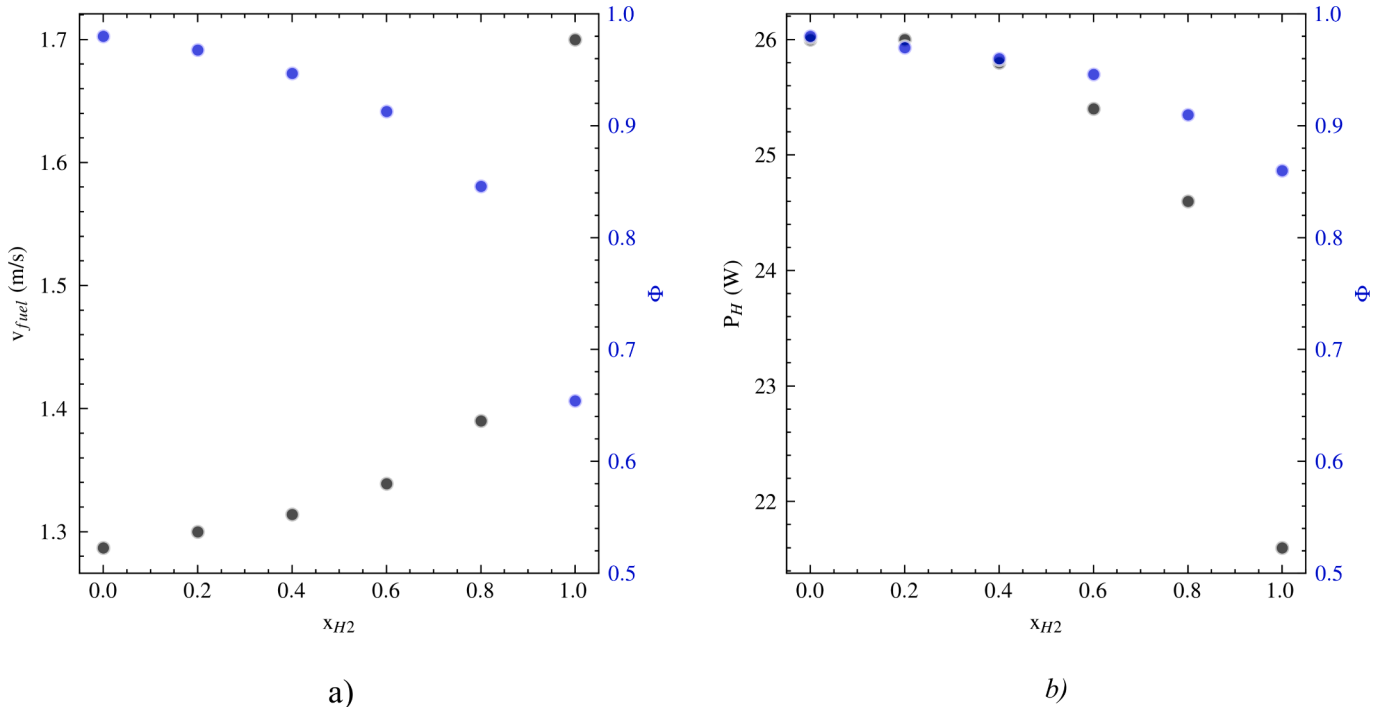


Fig. 4. Simulated test scenarios a) Constant thermal power $P_H=26$ W, b) Constant fuel velocity $v_{fuel} = 1.29$ m/s.

and reaction simulations.

The heat transfer coefficient h_0 is 20 W/m²K. The thermal material properties of the quartz glass are C_p 750 J/kgK, ϵ 0.93, and λ 2 W/mK, respectively. Fig. 4 presents test cases designed to examine the effects of varying hydrogen mole fraction (x_{H_2}) on combustion characteristics and MTPV efficiency. These tests are conducted under two specific conditions: a constant power output of 26 W (shown in Fig. 4a) and a constant volumetric flow rate (shown in Fig. 4b). By maintaining the fuel velocity (v_{fuel}) at 1.29 m/s, this study ensures that comparisons are strictly focused on the effects of the equivalence ratio (Φ) without interference from other operational parameters and Reynolds number (Re) effects.

2.5. Grid independence study and validation

The simulation mesh employs hexahedral cells, in the confluence zone—where fluid streams merge—prismatic cells are used to capture the geometry more accurately. To validate the simulation's reliability and ensure that results are not affected by the grid size, we conducted a detailed grid independence study with 56,000, 140,000, 175,000 and 237,000 cells. The grids were specifically refined in the flame zone to capture the complex phenomena occurring there. Fig. 5 displays the temperature distribution along the midline, providing visual insight into the effects of grid refinement.

The Grid Convergence Index (GCI) for the different mesh resolutions was calculated to estimate discretization errors, by established literature methodologies. Considering the temperature at the midline at an axial distance of 9 mm from the chamber inlet, the $GCI_{2/4}$ for the coarsest mesh is calculated to be 5.4 %, which exceeds the acceptable threshold and indicates a lack of convergence. For the 237,000-cell mesh, a $GCI_{1/2}$ of 0.2 % was attained, reflecting high precision in the simulation outcomes. Conversely, the 140,000-cell mesh exhibited a $GCI_{2/3}$ of 0.5 %, which is marginally higher but still acceptable for computational studies. Furthermore, the f^* value of 2364 K, extrapolated from the accuracy of the 175,000-cell intermediate mesh, suggested a predicted error rate of 0.5 % for the 175,000-cell mesh value (2350 K). This rate aligns with the 5 % confidence interval, underscoring the simulation's reliability. Consequently, this last mesh will be used in the subsequent studies.

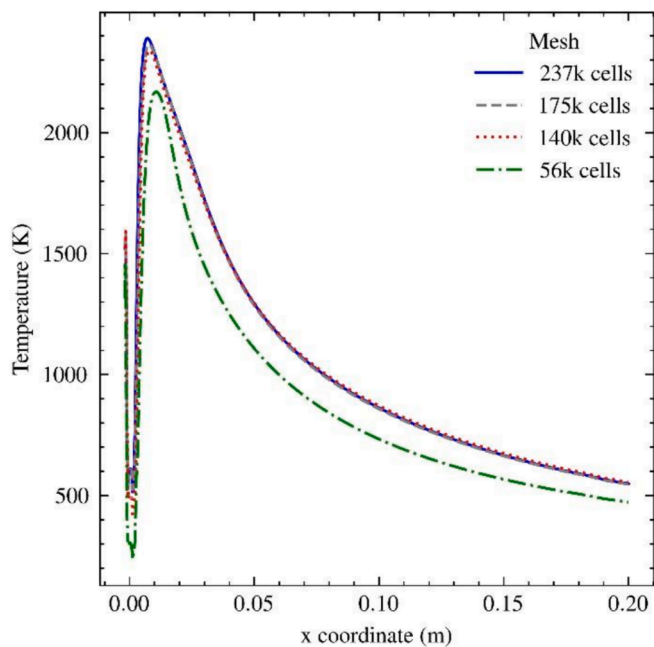


Fig. 5. Centerline temperature profile for $\Phi = 1$ at 298 K with H_2 /Air mixture across various grid refinements.

Notably, simulations indicated that stable flames could not be maintained for Φ values below 0.6, aligning with the experimental observations [62]. An OH mole fraction exceeding 0.2 was employed to accurately predict the numerical L_f . For $\Phi = 0.6$, the PMAC method shows an error of about 5 %, while the NB method has a significantly higher error of around 30 %. As Φ increases to 0.8, the errors for both methods increase, with NB showing a higher error of approximately 17 % and PMAC remaining lower at about 7 %. For $\Phi = 0.9$, both methods exhibit a reduction in error compared to the previous case, with PMAC at around 5 % and NB at about 10 %. At $\Phi = 1.0$, the PMAC method shows its lowest error, near 0 %, whereas the NB method maintains an error similar to that at $\Phi = 0.9$, around 10 %.

These data suggest that the PMAC method tends to produce lower errors compared to the NB method for all values of Φ considered. In particular, the PMAC method shows a decrease in error as Φ increases, with a minimum around $\Phi = 1.0$. The NB method, on the other hand, exhibits significant error at low Φ values, with a reduction in error for Φ greater than 0.6 but never achieving the accuracy levels of the PMAC method.

3. Results and discussion

Results are presented in an extensive comparative study on radiation models, exploring the impact of low hydrogen mole fractions x_{H_2} .

3.1. Effect of radiation modeling

The comparative analysis across Fig. 7a–c underscores the differential impact of incorporating various radiation models—NB and PMAC—alongside the effects of hydrogen mole fraction (x_{H_2}) variations on the thermal dynamics within the micro combustor. The NB model, focusing solely on the absorption effects of H_2O , typically predicts higher flame temperatures. In contrast, the PMAC model, which accounts for the absorption coefficients of additional species, shows more moderated flame temperatures and a relatively centralized flame positioning, suggesting a more stable and controlled combustion environment.

The distinction between these models becomes stark when viewed alongside the scenario without any radiation model, as depicted in Fig. 7c. In the absence of a radiation model, there is a marked rise in flame temperatures across the chamber, consistently exceeding 1200 K, highlighting the critical role of radiation effects in accurate thermal simulation. Without modeling these radiation effects, the system drastically overestimates temperatures, which could lead to significant design inefficiencies or operational challenges in MTPV systems.

As x_{H_2} increases from 0.05 to 0.2, the peak temperature zones shift toward the inlet of the combustion chamber, and the flame shape changes. This shift aligns with the higher combustion temperatures predicted by both the NB and PMAC models for increased hydrogen levels. The increase in x_{H_2} results in a more reactive fuel blend that burns more intensely and rapidly, moving the peak temperature zones and flame front closer to the inlet. Hydrogen's high flame speed and low ignition energy cause the flame to stabilize sooner, producing a hotter and more compact flame. The altered flame shape at higher x_{H_2} levels, which is more focused and intense, is due to hydrogen's ability to support faster and more complete combustion. This affects the flame's interaction with surrounding gas dynamics and chamber geometry, enhancing heat release near the inlet and modifying thermal gradients. These dynamics are critical in micro combustor designs for efficiency and stability, illustrating how fuel composition significantly impacts the combustion process and system performance. At an x_{H_2} of 0.05, a distinct variation in flame behaviour and temperature response is evident between the two radiation models, the PMAC and NB, as shown in the figure.

The PMAC model showcases a dynamic transition in the flame's shape, evolving from a U-shaped to an oblique flame profile as the

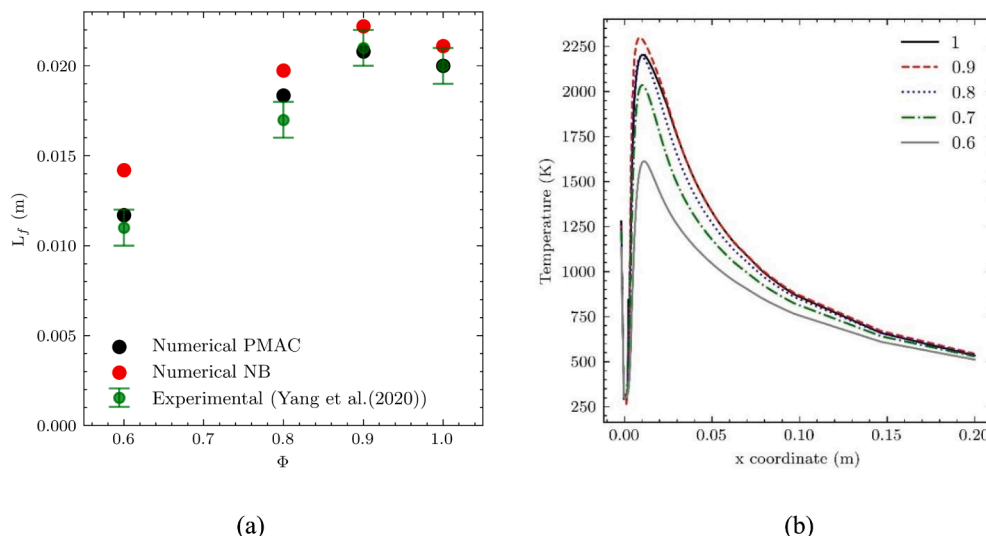


Fig. 6. a) validation for $x_{H_2} = 1$ flame length, b) PMAC midline temperature profile for different Φ .

hydrogen concentration increases.

In contrast, the NB model, which primarily considers H_2O in its radiation calculations, demonstrates a more consistent flame shape and temperature profile across different scenarios, including the low hydrogen concentration of $x_{H_2} = 0.05$.

The observed differences in flame shape and behaviour between the PMAC and NB models are attributable to how each model handles the absorption coefficients and the sensitivity to the concentrations of various species involved in the combustion. The NB model primarily focuses on H_2O as the dominant absorber in its radiative transfer calculations. This results in relatively consistent flame characteristics across different hydrogen concentrations because it focuses on a single species that exhibits a more linear response to changes in hydrogen levels. Conversely, the PMAC model includes a broader range of species such as NH_3 , NO , and OH in addition to H_2O , which significantly influences the combustion dynamics, especially at lower hydrogen concentrations. Here, these additional species are proportionally more impactful, altering both the thermal radiation and the flame dynamics. This results in noticeable changes in the flame's position and morphology, particularly evident at lower hydrogen levels where the relative concentration of these minor species compared to hydrogen is higher. As hydrogen concentration increases, the influence of these additional species in the PMAC model becomes less dominant because the increase in H_2 and the resultant H_2O from combustion dilutes their effects. This leads to a reduction in the variability of flame shape and behaviour at higher hydrogen concentrations, indicating a transition to a more H_2O -dominated regime. This comparison underscores the importance of choosing a model that accurately reflects the chemical dynamics of the fuel mixture being used, particularly in scenarios involving blended fuels where interactions between multiple species significantly affect combustion outcomes.

Fig. 8 presents the symmetry plane midline incident radiation and absorption coefficients for different x_{H_2} using the PMAC and NB models. In Fig. 8a, the incident radiation profiles under the PMAC model for varying x_{H_2} values (0.05, 0.1, 0.15, 0.2) indicate that higher hydrogen content significantly influences radiation intensity. At $x_{H_2} = 0.05$, the peak incident radiation reaches approximately $7.5 \times 10^5 \text{ W/m}^2$, whereas at $x_{H_2} = 0.2$, the peak decreases to about $4.0 \times 10^5 \text{ W/m}^2$. This decrease and shift toward the inlet suggest that with more hydrogen, the combustion process becomes more efficient, leading to less radiative heat loss. A similar trend is observed in Fig. 8b with the NB model, where the highest peak at $x_{H_2} = 0.05$ is around $6.8 \times 10^5 \text{ W/m}^2$, decreasing to roughly $3.8 \times 10^5 \text{ W/m}^2$ at $x_{H_2} = 0.2$. However, the differences between

various x_{H_2} levels are less pronounced in the NB model, indicating that while the NB model captures the general trend, it may not account for all species interactions affecting radiative transfer.

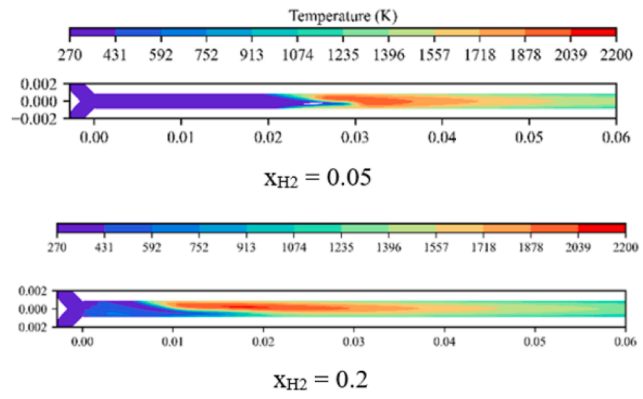
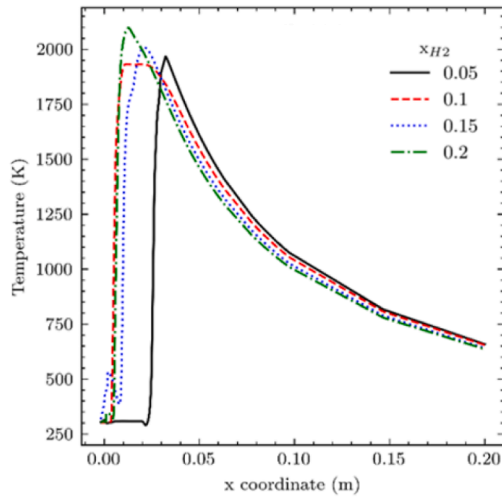
The absorption coefficient profiles for different x_{H_2} values in the PMAC model (Fig. 8c) reveal more detailed variations along the combustion chamber. At $x_{H_2} = 0.05$, the absorption coefficient starts high at around 0.35 1/m and decreases along the x-coordinate, whereas higher hydrogen fractions ($x_{H_2} = 0.1, 0.15, 0.2$) show less variation, with absorption coefficients ranging from approximately 0.2 to 0.25 1/m, indicating a more uniform absorption behavior. This suggests that with more hydrogen, the combustion zone becomes more homogeneous, reducing localized variations in absorption. In contrast, Fig. 8d shows that the absorption coefficient profiles under the NB model display a much narrower range of values, with absorption coefficients peaking around 0.003 1/m and remaining relatively flat across the x-coordinate for all x_{H_2} levels. This uniformity indicates that the NB model may not capture the detailed interactions between different species affecting absorption, reflecting its focus on water vapor as the primary absorber.

Fig. 9 showcases the OH mole fraction profiles along the symmetry plane midline for two different hydrogen mole fractions.

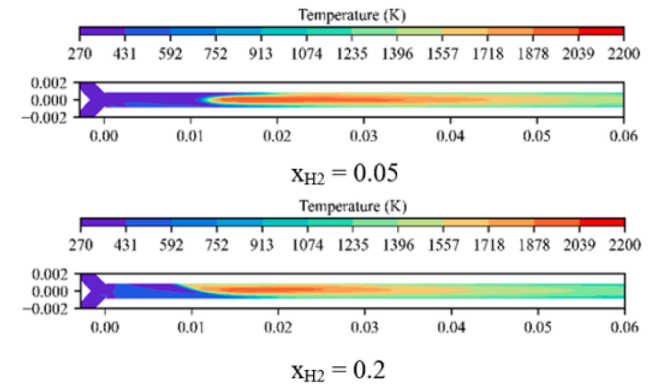
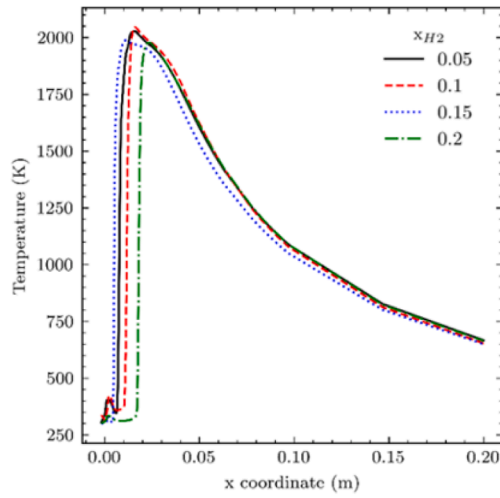
At $x_{H_2} = 0.05$, the PMAC model predicts a sharp peak in OH concentration near the inlet, with the peak value reaching approximately 0.0025. This peak rapidly declines, suggesting a quick initiation and a steep reduction in reactive zones. This peak is more pronounced compared to the NB model, which shows a peak value of about 0.0020. The NB model's peak is broader and extends further along the combustion chamber, indicating a less localized but more evenly spread combustion zone. The scenario without radiation modeling (W/O) shows a significantly dispersed OH mole fraction along the chamber with a peak value of around 0.0023, indicating an overestimation of the flame spread and lower confinement of the combustion zone.

At $x_{H_2} = 0.2$, the overall OH concentrations are higher, reflecting increased reactivity due to the higher hydrogen content. The PMAC model again shows a sharp peak, reaching about 0.0024, closely followed by the NB model with a peak of approximately 0.0021. Both models indicate effective utilization of the reactive mixture at higher hydrogen levels, with the PMAC model capturing a more acute peak, suggesting a better performance in high-temperature combustion dynamics. The W/O model displays a broader peak with a value around 0.0020, further indicating the importance of radiative heat transfer modelling for accurate prediction of combustion behaviour.

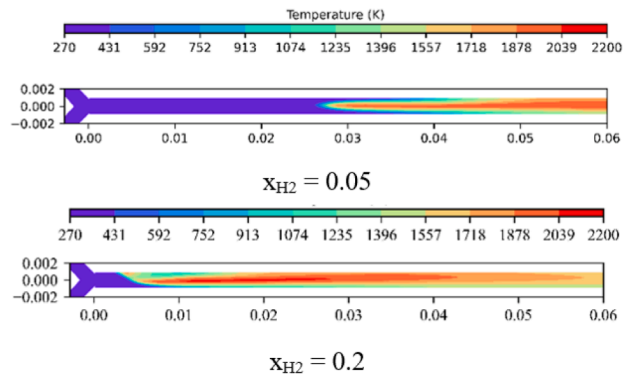
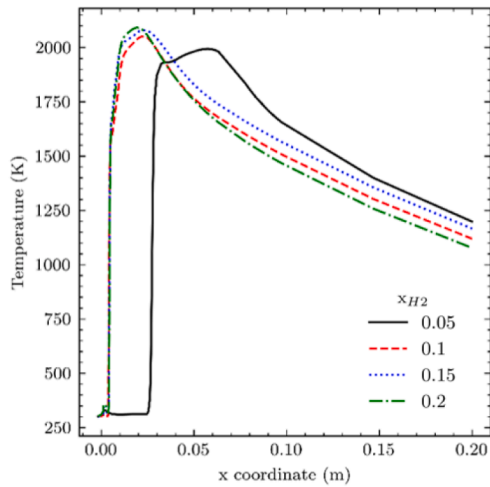
These observations align with the trends seen in Fig. 8a and b, where the PMAC model showed higher incident radiation and more detailed



a)



b)



c)

Fig. 7. Symmetry plane midline temperature and contours for a) PMAC, b) NB, c) W/O Radiation model.

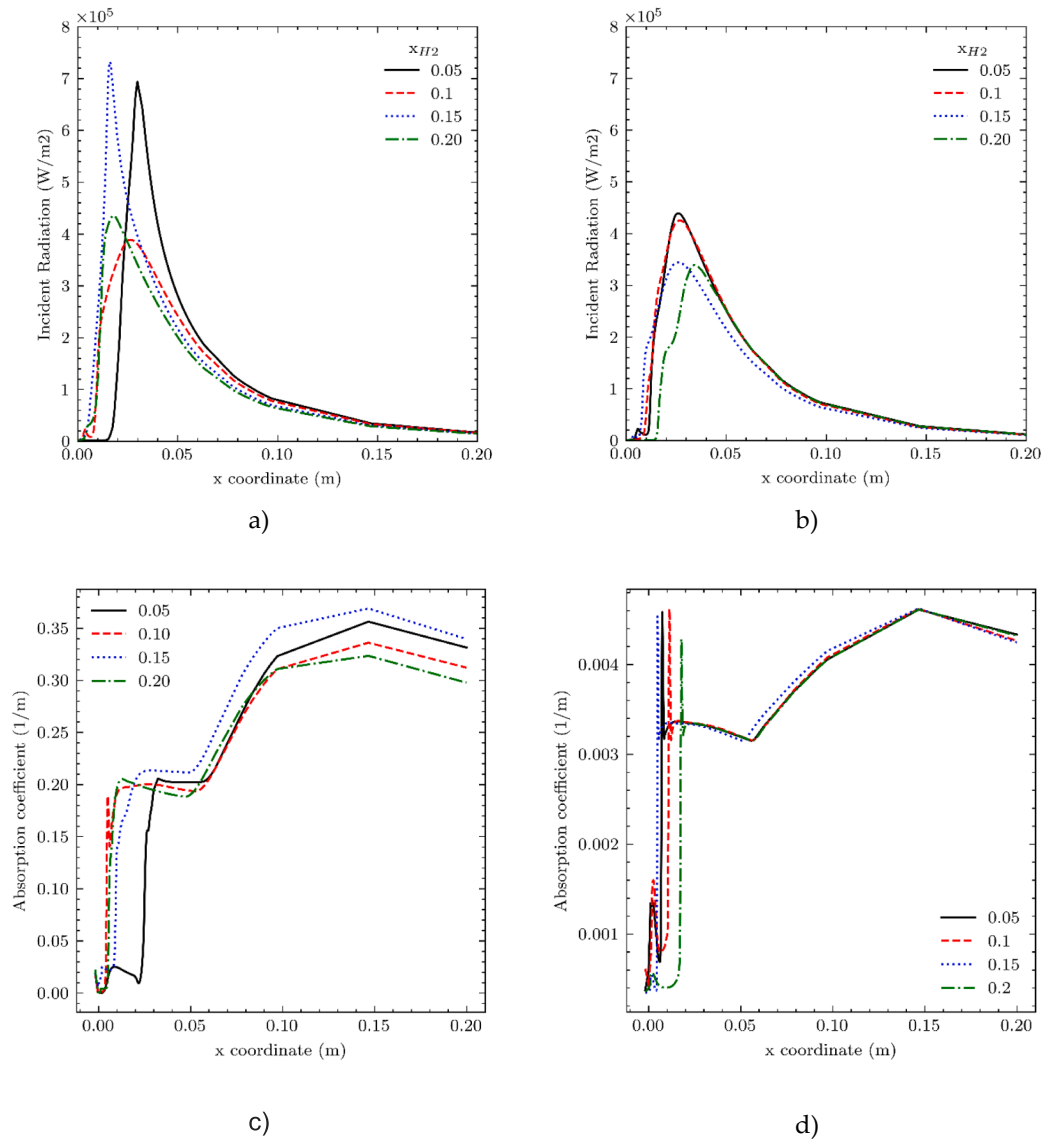


Fig. 8. Symmetry plane midline incident radiation and absorption coefficients for different x_{H_2} : a) PMAC model incident radiation, b) NB model incident radiation, c) PMAC model absorption coefficient, d) NB model absorption coefficient.

absorption characteristics, indicating its effectiveness in capturing the complex interactions of multiple species and their impact on combustion dynamics. The NB model, while less detailed, still provides a reasonable approximation but spreads the reactive zones more broadly, reflecting its focus on water vapor as the primary absorber.

Fig. 10 illustrates the NO mole fraction distributions along the symmetry plane for $x_{H_2} = 0.2$ across three different modeling scenarios: PMAC, NB, and without radiation (W/O Radiation).

The PMAC model shows a high concentration of NO near the inlet, with the peak concentration reaching approximately 0.0023, which sharply diminishes with increasing distance from the inlet. This sharp decline indicates that the PMAC model effectively captures the high-temperature zones conducive to NO formation, suggesting precise representation of chemical kinetics and localized thermal gradients, crucial for accurate NO prediction.

In contrast, the NB model exhibits a broader distribution of NO, with a peak concentration of around 0.0019. This spread indicates a less intense peak concentration compared to the PMAC model. The broader NO profile suggests that while the NB model accounts for heat transfer, its focus on H₂O as the primary radiative agent might limit its ability to

capture the precise, high-temperature peaks that promote concentrated NO formation. The more distributed NO profile in the NB model could indicate a more uniform thermal environment along the duct, reflecting a less efficient peak temperature management.

The scenario without radiation modeling (W/O Radiation) shows an even more extended NO distribution, with the peak concentration around 0.0015, highlighting the critical role of radiative heat transfer in accurate combustion modeling. This model's inability to localize high-temperature zones results in dispersed and inefficient combustion, as evidenced by the widespread low concentrations of NO. This suggests that ignoring radiation effects can lead to significant inaccuracies in simulating combustion dynamics, particularly in the formation and distribution of combustion-related pollutants like NO.

3.2. Effect of fuel blending

The impact of fuel blending on combustion characteristics is examined in this section. Unless otherwise specified, all analyses and values are based on simulations at constant P_H (Fig. 4a).

The impact of fuel blending on combustion characteristics is

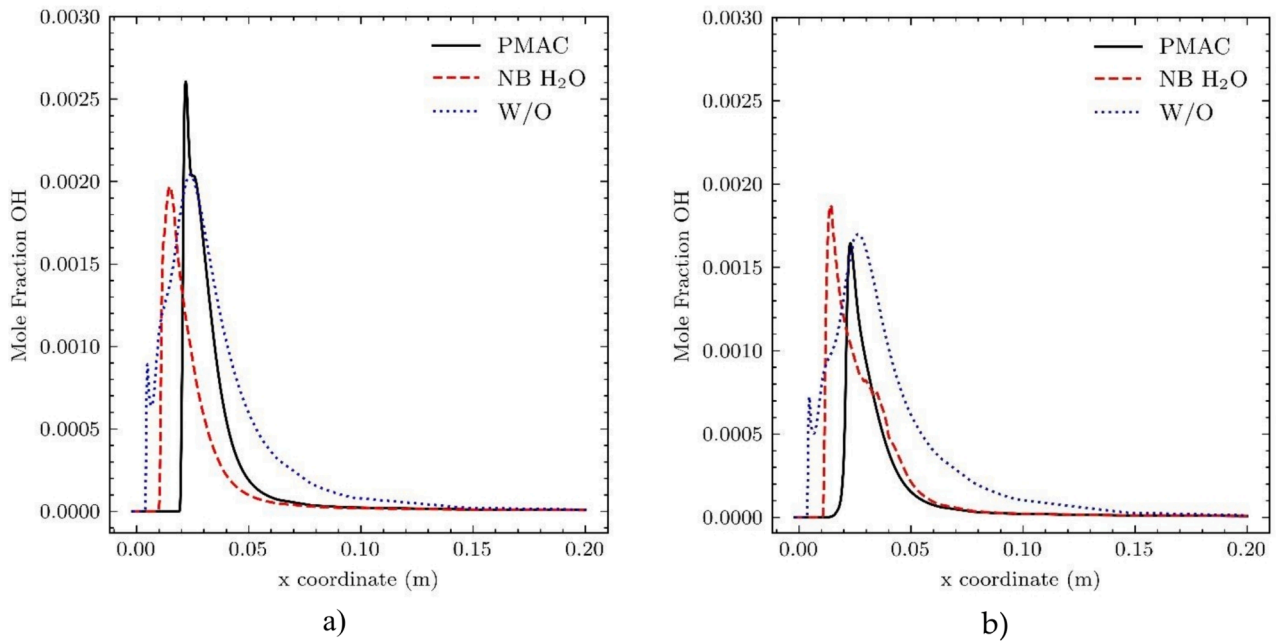


Fig. 9. OH Mole Fraction Along the Symmetry Plane Midline (a) $x_{H_2} = 0.05$; (b) $x_{H_2} = 0.2$.

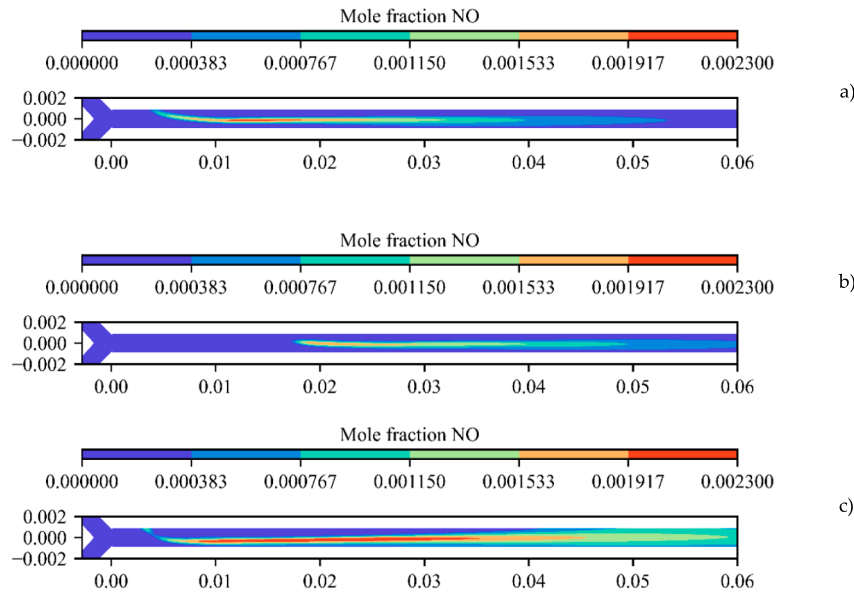


Fig. 10. $x_{H_2} = 0.2$ symmetry plane NO mole fraction for a) PMAC, b) NB, c) W/O Radiation.

illustrated in Fig. 11, which consists of two parts: (a) the symmetry plane midline temperature at different hydrogen mole fractions (x_{H_2}), and (b) the relationship between the maximum flame temperature and its corresponding x coordinate.

In Fig. 11a, the midline temperature profiles for various x_{H_2} values (ranging from 0 to 1.0) are shown. As x_{H_2} increases, there is a noticeable decrease in peak temperature, and the location of this peak shifts closer to the inlet. This trend indicates a hyperbolic relationship where higher hydrogen content facilitates quicker ignition, thereby lowering the overall peak temperature due to the more efficient heat transfer to the chamber walls.

Fig. 11b provides a comparative analysis of the maximum flame temperature and its corresponding x coordinate for both constant P_H (black marks) and constant v_{fuel} (red marks) scenarios. As x_{H_2} increases,

the maximum temperature decreases and the location of this maximum shifts toward the inlet. For $x_{H_2} = 0$, the flame exhibits a U-shaped structure with the peak temperature further downstream. However, at higher x_{H_2} values, the flame becomes asymmetrical, reflecting the efficient heat transfer properties of hydrogen.

The red and black markers in Fig. 11b highlight the differences between constant P_H and constant v_{fuel} cases. In constant P_H scenarios (black), the peak temperatures and their locations vary less significantly compared to constant v_{fuel} cases (red), where the impact of hydrogen content is more pronounced. This indicates that maintaining a constant power output results in more stable flame characteristics despite changes in fuel composition.

Fig. 12 further elucidates these trends by presenting the flame temperature distribution at different x_{H_2} values. The images clearly show

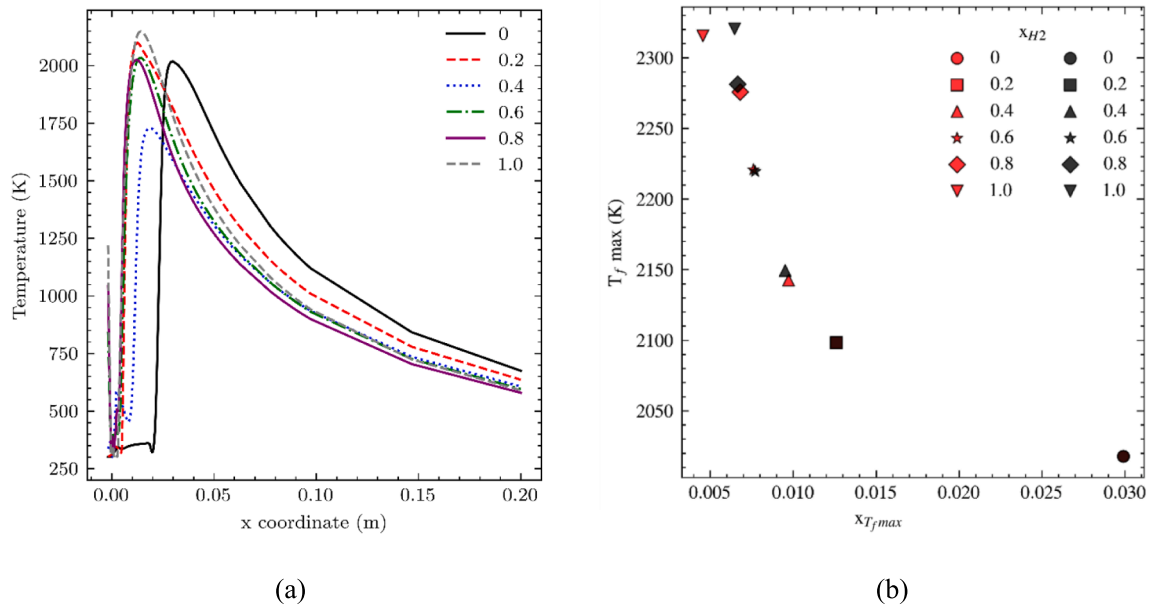


Fig. 11. A) symmetry plane midline temperature at different x_{H_2} , b) $T_f \text{ max}$ vs x coordinate for P_H (black) and v_{fuel} (red) constant cases. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

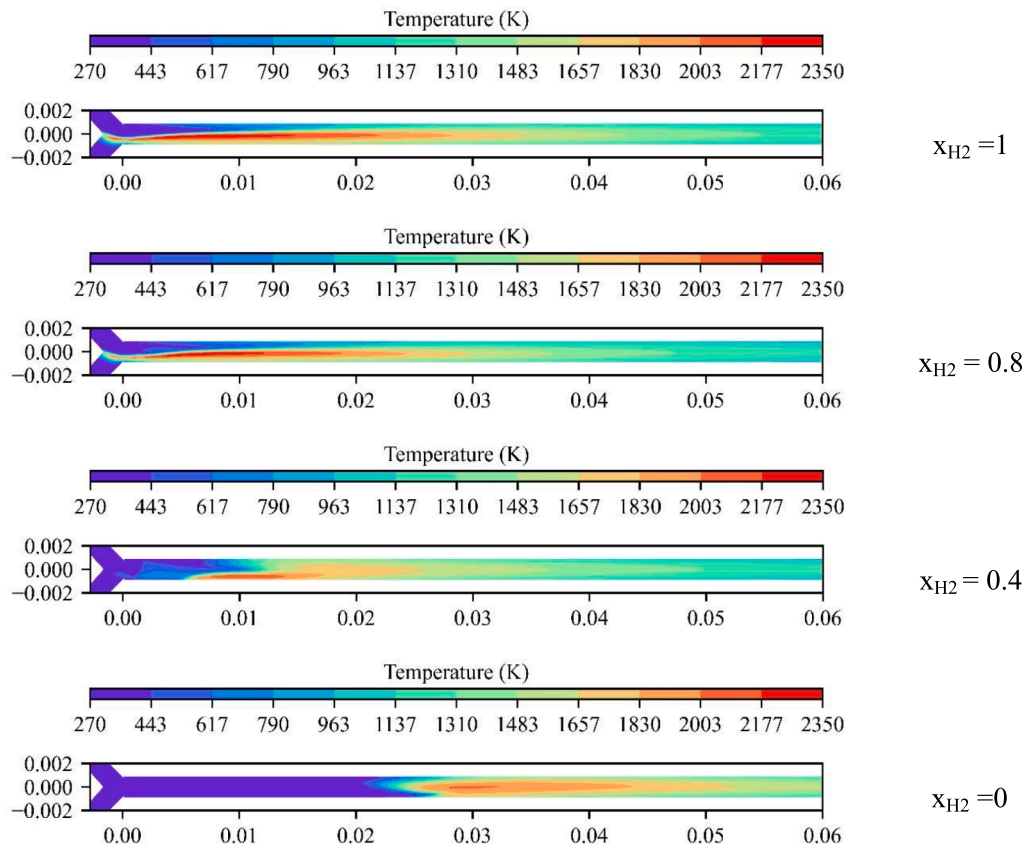


Fig. 12. Flame temperature at different x_{H_2} .

that increasing x_{H_2} results in a significant shift of the high-temperature region towards the inlet. Specifically:

At $x_{H_2} = 0$, the flame shows a more dispersed temperature profile, indicating a broader combustion zone. At $x_{H_2} = 0.4$ and 0.8 , the high-temperature regions become more concentrated and shift closer to the

inlet, reflecting more efficient combustion and heat transfer. Finally, at $x_{H_2} = 1.0$, the flame temperature distribution is highly concentrated near the inlet, demonstrating the maximum efficiency in heat transfer and combustion with pure hydrogen.

Fig. 13 illustrates the impact of varying hydrogen mole fractions on

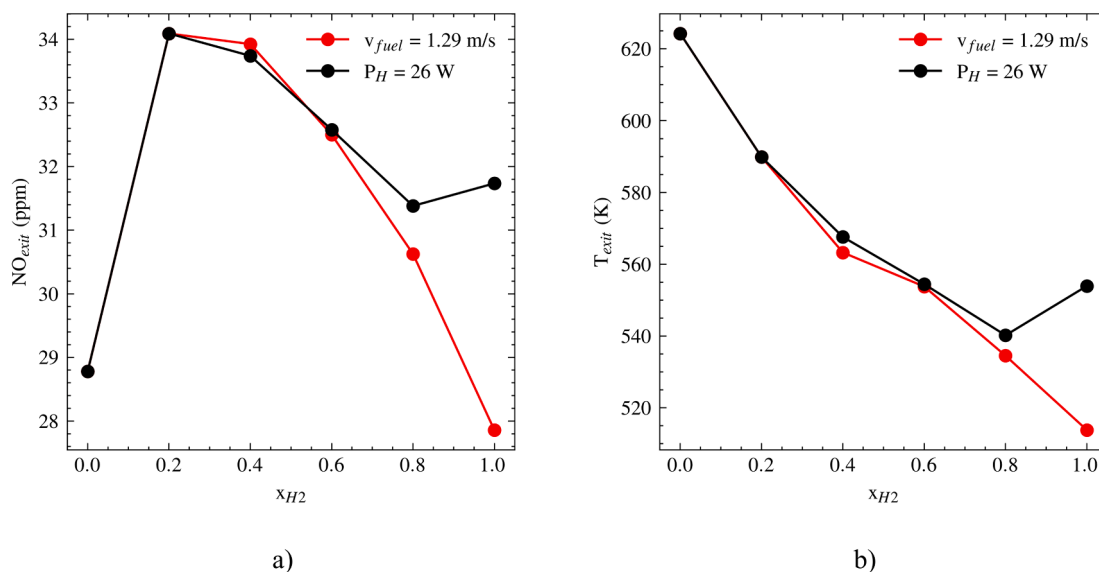


Fig. 13. P_H and v_{fuel} constant cases a) NO_{exit} , b) T_{exit} .

NO emissions at the exit and temperatures under different scenarios. NOx refers to the combined concentration of NO and NO_2 , as the interconversion between these two species occurs rapidly in both the stratosphere and troposphere. The NO concentration is found to be three orders of magnitude higher than that of NO_2 in all test cases, as documented by ammonia combustion literature [67]. Therefore, only the NO mole fraction will be investigated, and NO will be considered synonymous with NOx. In the context of the microcombustor, the typical temperature ranges observed are high (e.g., peak temperatures exceeding 2000 K), which favor the formation of NO primarily through the thermal NO mechanism. The specific conditions in the microcombustor—such as high temperatures, pressure, and the presence of oxygen—promote the rapid formation of NO while inhibiting the significant formation of other nitrogen oxides like NO_2 , N_2O , N_2O_3 , and N_2O_4 . Therefore, given the high temperatures and efficient combustion conditions in the microcombustor, NO is the predominant nitrogen oxide formed. Lower temperatures and different chemical environments would be required to see substantial concentrations of the other nitrogen oxides.

In Fig. 13a, the NO mole fraction at the exit (NO_{exit}) is shown as a function of x_{H_2} . The NO concentration peaks at x_{H_2} values of 0.2 and 0.4, reaching around 34 ppm. It then significantly decreases, with the lowest values observed at $x_{H_2} = 0.8$ for constant P_H (29 ppm) and $x_{H_2} = 1.0$ for the constant v_{fuel} cases (27 ppm). This decrease is more pronounced in the constant fuel velocity scenarios. This trend suggests an effective deNOx effect facilitated by the presence of ammonia, which interacts with the available oxygen to reduce NOx formation, particularly at higher hydrogen concentrations.

Fig. 13b shows T_{exit} as a function of x_{H_2} . Both trends demonstrate a general decrease in T_{exit} , which helps explain the NO_{exit} behavior as a result of the interplay between mixture composition, ammonia concentration, flame position, equivalence ratio (Φ), and temperature. At an equivalence ratio of 0.4, the lean mixture results in higher NO values compared to richer conditions, likely due to the behaviour of ammonia in the presence of excess oxygen atoms. Ammonia, when not fully combusted, can effectively reduce NOx emissions by reacting with NOx to form nitrogen and water, especially at lower temperatures and lean conditions. This collectively indicates that increasing x_{H_2} in the fuel blend significantly influences NOx emissions and exit temperatures. Higher hydrogen content tends to reduce both NOx emissions and exit temperatures, promoting more efficient and cleaner combustion. The observed trends also underscore the importance of balancing mixture

composition and operational parameters to optimize performance and minimize emissions.

Fig. 14a and b illustrate the reaction rates for NO formation pathways along the symmetry plane midline at $x_{H_2} = 0.2$ (a) and $x_{H_2} = 1$ (b). In Fig. 14a, the graph indicates that the R6 reaction dominates, suggesting that the HNO pathway is the primary contributor to NO production within the flame zone. On the other hand, in Fig. 14b, the R1 and R6 reactions are both significant within the flame area. This finding points to the thermal NO formation pathway becoming comparably important in the production of pollutants, and it occurs at a rate that is two orders of magnitude faster than the HNO pathway observed in the $x_{H_2} = 0.2$ scenario.

The substantial increase in the reaction rate of the thermal NO pathway in the pure H_2 scenario is indicative of the complex chemistry involved in NO production. The associated reactions are detailed in Table 3, which provides the nomenclature and specifics of each reaction pathway involved in the formation of NO.

These findings demonstrate how different hydrogen mole fractions influence the NO formation mechanisms, with thermal NO becoming increasingly significant at higher hydrogen concentrations due to elevated temperatures and enhanced reaction kinetics. This underscores the importance of detailed chemical kinetic modeling to accurately predict NO emissions under varying fuel compositions.

3.3. Effect of equivalence ratio

The outer average wall temperature ($T_{we, mean}$) is illustrated in Fig. 15. The MTPV emission plane has been segmented into three distinct sections to effectively demonstrate the temperature distribution and the resulting radiative power variations as a function of x_{H_2} . It is evident from the data that an increase in hydrogen concentration leads to a higher average temperature in the section with x coordinate < 3 cm of the emission plane. Specifically, at $x_{H_2} = 1.0$, the temperature in this section reaches approximately 1100 K, compared to about 900 K at $x_{H_2} = 0$. In contrast, with higher NH_3 concentration, there is a noticeable increase in temperature in the other sections, particularly in the sections with x coordinate > 3 cm. This phenomenon can be attributed to the flame position being significantly further downstream, causing the heat to distribute more uniformly along the emission plane.

The points (without connecting lines) represent the average temperature across the entire surface of the emission plane, rather than in specific sections. These points provide a comprehensive view of the

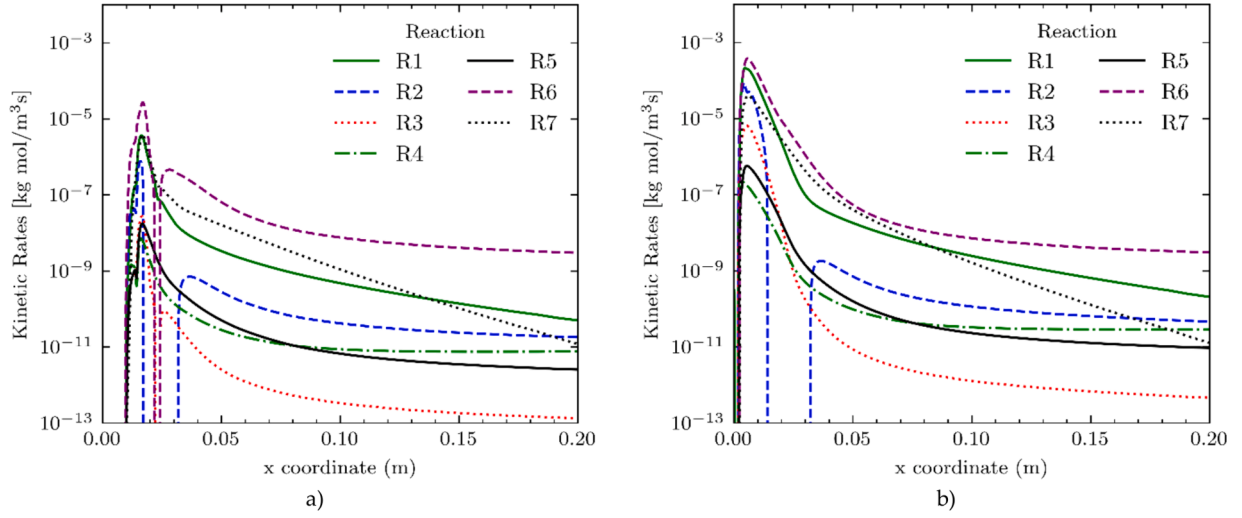


Fig. 14. Reaction Rates of NO Pathways Along Symmetry Plane Midline (a) $x_{H_2} = 0.2$, (b) $x_{H_2} = 1.0$.

Table 3

Main NO Path Reactions.

Reactions of NO Path			
R1	$N + O_2 = NO + O$	R5	$NH_2 + NO = NNH + OH$
R2	$N + OH = NO + H$	R6	$HNO + OH = NO + H_2O$
R3	$NH + O = NH + H$	R7	$HNO + O_2 = NO + HO_2$
R4	$NH_2 + NO = N_2 + H_2O$		

overall thermal behavior of the system. It can be observed that the average surface temperature is relatively stable, with slight fluctuations corresponding to different x_{H_2} values. For example, the average temperature for the entire surface ranges from approximately 600 K to 800 K across the different hydrogen concentrations, indicating a general trend of increasing temperature with higher x_{H_2} values.

This nuanced behaviour underscores the complex interplay between fuel composition and thermal dynamics within the MTPV emission system efficiency. By comparing cases, it is evident that under leaner conditions (Fig. 15b), the average temperatures are generally lower. The temperature profiles indicate a drop in temperature as the hydrogen

concentration decreases, emphasizing that leaner mixtures result in lower overall temperatures, which correlates with reduced radiative power and efficiency in the MTPV system. These trends highlight the importance of optimizing fuel composition to balance between achieving high emitter temperatures for efficient power conversion and maintaining overall system stability and efficiency.

Fig. 16 illustrates the temperature and NO mole fraction along the symmetry plane midline for $x_{H_2} = 1.0$. In the temperature profile (Fig. 16a), the higher fuel velocity of 1.7 m/s shows a higher peak temperature compared to 1.29 m/s. This is because the increased velocity leads to a more vigorous mixing and combustion process, resulting in higher localized temperatures. The NO mole fraction profile (Fig. 16b) follows a similar trend, with the higher velocity case showing a higher NO concentration near the inlet. This correlation between temperature and NO concentration is expected, as NO formation is strongly temperature-dependent.

Fig. 17 complements these findings by presenting the NO concentration contours for both fuel velocities at $x_{H_2} = 1.0$. In Fig. 17a, with $v_{fuel} = 1.7$ m/s, the NO concentration exhibits a broader and more pronounced distribution, indicating a more efficient combustion process

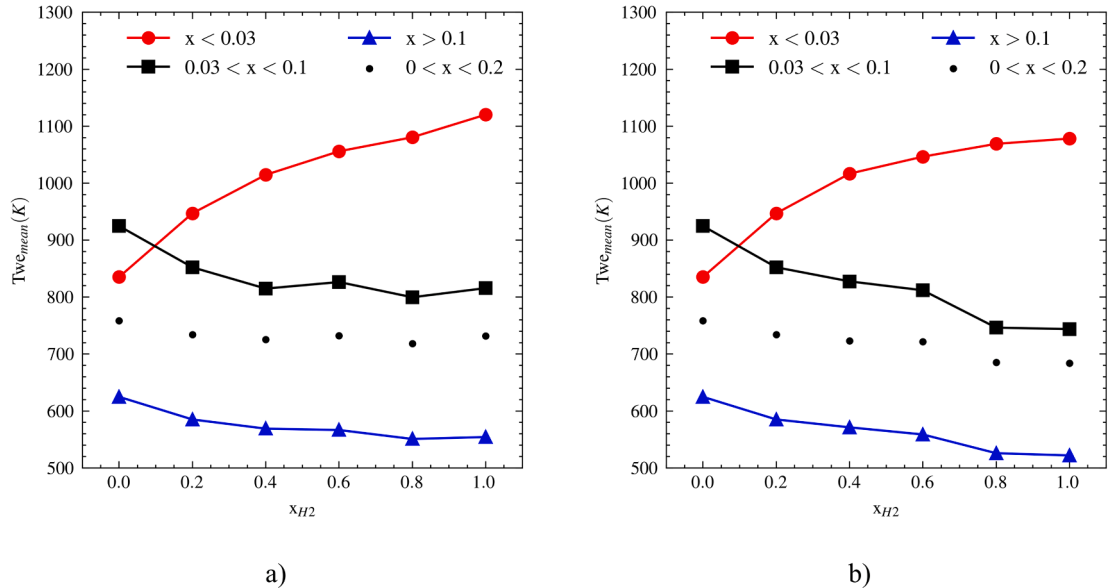


Fig. 15. $T_{w,mean}$ at constant a) P_H , b) v_{fuel} .

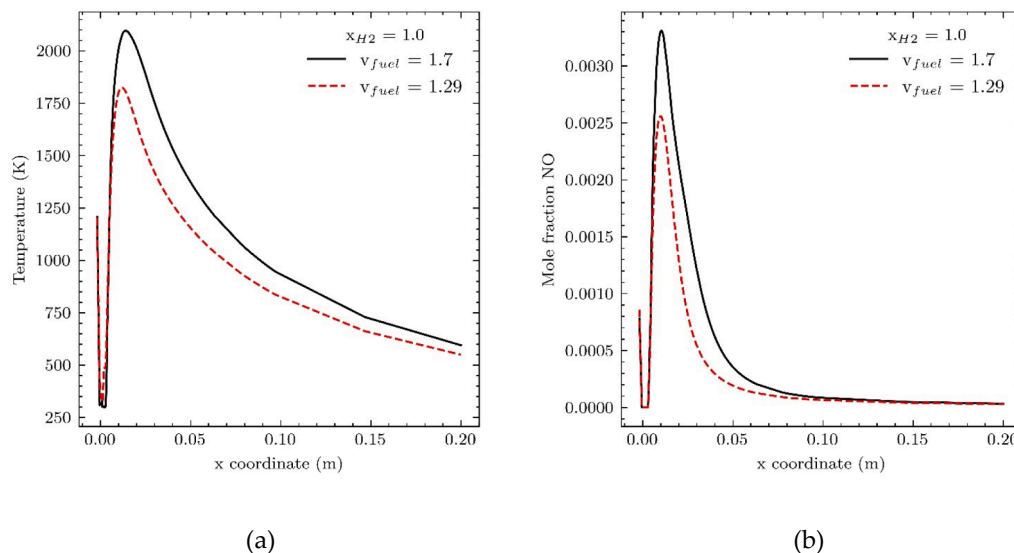


Fig. 16. Symmetry plane midline $x_{H_2} = 1.0$ for a) temperature, b) NO mole fraction.

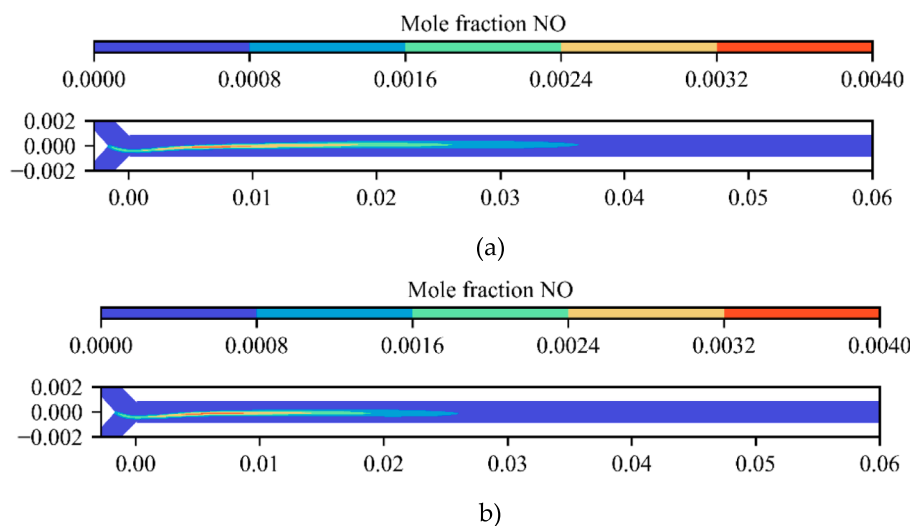


Fig. 17. NO Mole fraction $x_{H_2} = 1.0$ a) $v_{fuel} = 1.7$ m/s, b) $v_{fuel} = 1.29$ m/s.

with higher temperatures and enhanced NO formation. In contrast, Fig. 17b ($v_{fuel} = 1.29$ m/s) shows a more confined NO distribution, reflecting the lower peak temperatures observed in the temperature profile.

These observations highlight the impact of fuel velocity on the combustion characteristics within the MTPV device. The higher fuel velocity enhances mixing, leading to higher peak temperatures and NO concentrations, which subsequently affect the thermal efficiency and emission profiles of the system. The interplay between temperature distribution and NO formation underscores the importance of optimizing fuel velocity to balance efficient combustion with controlled pollutant emissions.

3.4. Radiation efficiency analysis

The final analysis of the MTPV system efficiency focuses on different fuel blends and their impacts on system performance. MTPV system efficiency relies on the spectral quality of radiation heat and the

temperature differential between the emitter and the photovoltaic cells. In combustion-driven MTPV systems, managing wall temperature is critical. Elevated wall temperatures can yield a stable thermal emitter profile, potentially improving MTPV conversion efficiency. However, the emitter panel's surface area is also crucial, as a larger area can radiate more thermal energy, providing more power for the MTPV cells to convert into electricity [65]. The interrelation between the emitter panel's temperature and surface area is pivotal in optimizing the system's overall efficacy. The device under analysis has a substantial surface area relative to its cross-sectional area, significantly impacting system efficiency. It is essential to determine whether the local wall temperature elevation due to hydrogen combustion is balanced by subsequent energy losses.

Notably, the Y-shaped design continues to be one of the most effective configurations for microscale MTPV applications, offering a balance between heat management and efficient energy conversion [64,69,70]. The pertinent area refers to the region within the MTPV system that is directly affected by radiative heat transfer. This area is crucial for the

system's efficiency as it determines the interaction between the emitted thermal radiation and the photovoltaic cells. In this study, the pertinent area is defined by the dimensions of the mixing chamber in the XY plane, which measures 2 mm by 200 mm ($4 \times 10^{-4} \text{ m}^2$). Analysing the mean outer wall temperature is essential to assess the thermal behavior of the micro combustor effectively. This parameter serves as a quantifiable index to gauge the average temperature along the outer wall and is a key indicator [63].

Photovoltaic cells and MTPV emitter wall spacing is an important parameter for MTPV microsystems. According to Bani et al., the efficiency of the MTPV system η drops from 18 % to 8.5 % when the distance increases from 1 mm to 6 mm [69]. However, this factor can be considered negligible if the distance between the wall and the photovoltaic cell is less than 1 mm, which has been assumed in this study. The radiation efficiency η is defined by the ratio of the radiative power output (P_R) to the fuel input power, as described by the following equation [68,71]:

$$\eta = \frac{P_R}{P_H} = \frac{\varepsilon \sigma \sum_{i=1}^n A_{we,i} (T_{we,i}^4 - T_0^4)}{\dot{m}_{fuel} \text{LHV}} \quad (8)$$

Where $A_{we,i}$ is mesh cell area, quartz emissivity $\varepsilon = 0.93$, σ Boltzmann's constant, $T_{we,i}$ and T_0 the temperature of the outer wall and photovoltaic panel equal to the ambient temperature, 300 K. With higher x_{H2} potentially leading to augmented wall heat losses, this may negatively impact the performance.

Considering the $x_{H2} = 1$ validation cases (Fig. 6a), Fig. 18 shows the trends of η and the P_R as Φ varies. The radiant power follows the temperature and flame length function, reaching a maximum radiant power of 10.4 W at $\Phi = 0.9$ and radiant efficiency equal to 42.1 %. The η trend shows that the most inefficient condition is at $\Phi = 1$ (38.1 %).

Fig. 19 presents η (depicted as bars) and radiant power P_R (represented by lines) as functions of x_{H2} under two conditions: constant thermal power, shown in black, and constant fuel velocity, shown in red. P_R remains relatively stable across different x_{H2} , with only slight variations. For both scenarios the radiative power values range from approximately 8.5 W to 10 W, indicating consistent performance of the MTPV system in terms of radiative power output irrespective of the fuel blend.

The efficiency exhibits slight fluctuations as x_{H2} varies. For the constant P_H scenario (black line), the efficiency generally maintains around 32–34 %, showing minor dips at intermediate x_{H2} values. For the constant v_{fuel} scenario (red line), the efficiency displays a similar trend but starts lower than the constant P_H scenario, with values ranging from approximately 27 % to 31 %. The efficiency is slightly lower at higher

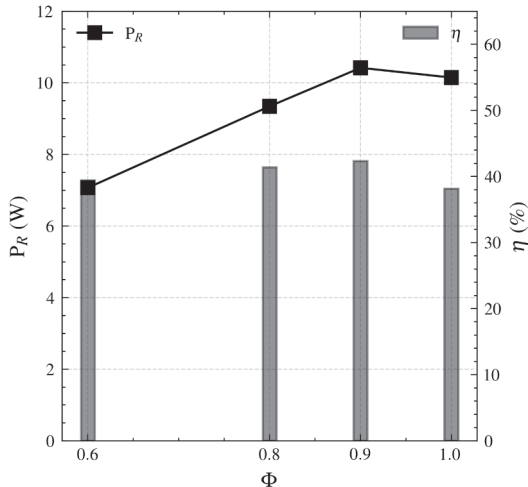


Fig. 18. P_R and η for vs Φ for $x_{H2} = 1$ condition.

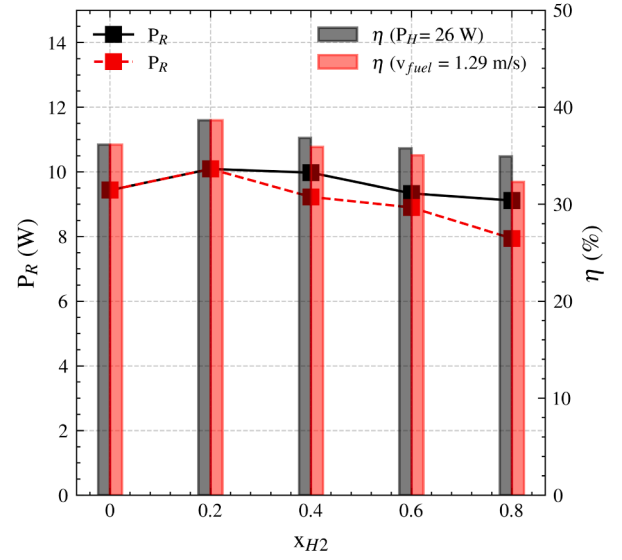


Fig. 19. P_R and η for vs x_{H2} for P_H (black) and v_{fuel} (red) constant cases. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

x_{H2} values (x_{H2} equal to 0.6 and 0.8).

The efficiency under constant P_H conditions is consistently higher than under constant v_{fuel} conditions. This suggests that maintaining a constant power output is more effective in optimizing the efficiency of the MTPV system. The variations in P_R and η are less pronounced under constant P_H conditions, indicating a more stable performance compared to the constant v_{fuel} scenario.

As x_{H2} increases from 0 to 0.2, P_R increases from about 9.4 W to approximately 10.1 W under both conditions, indicating enhanced combustion and effective radiative heat transfer. The radiation efficiency also shows an initial increase, suggesting better conversion of thermal energy to radiative power.

However, as x_{H2} increases from 0.2 to 0.8, P_R stabilizes around 9.1 to 9.9 W. This is due to the peak temperature shifting closer to the inlet, leading to a more localized high-temperature zone. This reduces the overall area of high temperature along the combustion chamber, impacting on the radiation efficiency. The elevated peak temperatures near the inlet cause higher thermal losses, reducing overall efficiency. Additionally, the reduction in the effective radiative area means less energy is converted to radiative power, despite higher peak temperatures.

In summary, while an initial increase in hydrogen content improves radiative power output and efficiency due to enhanced combustion dynamics, further increases beyond x_{H2} of 0.2 lead to diminishing returns. The shift of the high-temperature zone towards the inlet and the reduction in the overall high-temperature area, combined with increased thermal losses, result in a decrease in efficiency.

The overall analysis highlights that while the radiative power output is relatively stable across different hydrogen mole fractions, the efficiency is slightly more variable, particularly under constant fuel velocity conditions. This suggests that the fuel composition and operational parameters must be carefully managed to optimize the MTPV system's performance and efficiency.

Table 4 present MTPV efficiencies for same fuel mixtures in literature versus the present results, knowing that this work is the first MTPV study for blending H_2/NH_3 /air.

As observed, the order of magnitude of the radiation efficiency of these devices with hydrogen and ammonia is around 40 %, and our H_2/NH_3 /air MTPV has η comparable to other mixtures and design in literature (Table 4). Moreover, the increase in flow rate and hydrogen

Table 4MTPV literature studies mixture and η range.

Authors	Mixture (fuel-oxyder)	η (min–max) %
This study	NH ₃ /H ₂ /O ₂ -N ₂	32–39
Bani et al. [69]	H ₂ -O ₂	32–47
Cai et al. [71]	NH ₃ /H ₂ /O ₂	31–38
Zuo et al. [16]	H ₂ /O ₂ -N ₂	32–46
Luo et al. [29]	NH ₃ /H ₂ /O ₂	55–63
Li et al. [18]	H ₂ /O ₂ -N ₂	35–40

concentration does not always lead to an increase in efficiency, with an optimum blending solution varying x_{H_2} between 10 % and 40 % in literature. Cai et [74] investigated a planar premixed MTPV for an NH₃/H₂/O₂ mixture demonstrating that increasing the hydrogen molar fraction from 0 to 0.1 increases efficiency then to 35 % results in a lower outer mean wall temperature of the combustor, consequently leading to lower radiation efficiency. Luo et al. [29] in an NH₃/H₂/O₂ mixture found an increase of radiation efficiency with hydrogen contribution, mainly between x_{H_2} from 10 to 15 % with the most reasonable composition of 0.35.

The Table 5 below outlines the absorbed radiation fluxes and the radiation power for each test case.

In conclusion, considering the optimal x_{H_2} and Φ for a MTPV system involves balancing efficiency, stability, and safety. A moderate hydrogen molar fraction of 0.2 is generally suitable as it provides good radiative power without excessive harmful emissions. Lean combustion conditions are preferred to minimize Tmax generation to reduce thermal stress, but decrease radiant efficiency. For the case of pure hydrogen, the radiant power correlates with Φ with best condition at 0.9 and the efficiency increasing of 10 % from the leanest to the best condition. Pure hydrogen cases pose significant safety risks and thermal issues. Pure hydrogen can lead to explosion hazards and requires strict management of operating conditions to prevent accidents. Moreover, pure hydrogen scenarios can generate excessive heat, potentially damaging equipment and reducing operational efficiency. Therefore, it is preferable to opt for leaner conditions to mitigate these risks and ensure safer and more stable operations. While these suggested values provide a guideline, future work with new studies at different mass flow rates, Φ and and experimental data will be essential to fine-tune MTPV systems and applications.

4. Conclusions

This investigation aimed to assess the effect of radiation models on the performance prediction of a microcombustor for micro thermophotovoltaic (MTPV) applications. Specifically, the radiation model was characterized by evaluating the impact of a Narrow Band model with H₂O and a Planck Mean Absorption Coefficient model utilizing major species involved in hydrogen/ammonia/air combustion. The focus was on understanding how different radiation approaches influence the combustion process in microcombustion, energy efficiency, and pollutant production and if the radiation can be considered negligible. The second aim of this study was to investigate the effects of varying hydrogen concentrations on flame shape, temperature, NOx emissions and the radiant efficiency of the system.

Table 5TPV area Radiation Fluxes and P_R for P_H constant cases.

x_{H_2}	ϵ_f	Absorbed Radiation Flux (W)	P_R (W)
0	0	11.32	9.4
0.2	2.2	11.7	10.1
0.4	5.6	11.3	9.9
0.6	11.8	9.21	9.3
0.8	26.3	9.18	9.1

- Incorporating the absorption coefficients of ammonia and its products, the PMAC model consistently produced lower errors in flame length compared to the NB method across all equivalence ratios, with errors ranging from 0 % to 7 % for PMAC and 10 % to 30 % for NB, the lowest error occurring at $\Phi = 1.0$. Additionally, the prediction of laminar burning velocity (LBV) differed by approximately 4 % between the two models.
- The impact of the radiation model on the flame length prediction is significant at low hydrogen concentrations (x_{H_2} around 0.2–0.4)
- PMAC approach, compared to NB, impacts laminar burning velocity at inlet temperatures above 330 K with increased radiation losses of up to 4 % difference. For hydrogen concentrations above 0.4, the radiation losses result in a negligible difference in LBV.
- The Planck Mean Absorption Coefficient model accurately captures the transition of the steady flame shape from U-shaped to oblique with increasing hydrogen concentrations, aligning well with experimental results. It shows that as H₂ increases, the flame moves closer to the Y-shape intersection. Neglecting radiation significantly overestimates outlet and wall temperatures. In contrast, the water vapor Narrow Band model shows less variability in flame behavior across different blends, highlighting the importance of a multispecies approach.
- Increasing the hydrogen concentration leads to a rise in flame temperature and shifts the flame towards the inlet. Regarding NOx emissions, higher outlet emissions are observed at low hydrogen concentrations, between 0.2 and 0.4
- The radiative power remains relatively stable across different hydrogen mole fractions, with radiative power values ranging from approximately 8.5 W to 10 W and highest values at x_{H_2} around 0.2–0.4.
- Efficiency generally maintains around 32–34 % under constant power output and around 27–31 % under constant fuel velocity. Efficiency is slightly lower at higher x_{H_2} blends (x_{H_2} equal to 0.6 and 0.8) and with an observed increase in efficiency of 10 % when moving from the leanest condition to the optimal condition at an equivalence ratio of 0.9.

Concluding, a hydrogen molar fraction of 0.2 to 0.4 and an equivalence ratio (Φ) close to 0.9 appear to be most suitable for the microthermophotovoltaic (MTPV) system.

5. Fundings

The work was supported and funded by the PON R&I 2014-2020 Axis I "Investments in Human Capital" Action IV.5 "Innovative Doctorates on Green issues" - Doctorate Course in "Engineering of Complex Systems" XXXVII cycle - University of Salento" and "Finanziato dall'Unione europea - Next Generation EU". However, the views and opinions expressed are those of the authors alone and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them "PNRR - MISSION 4 - COMPONENT 2- INVESTMENT 1.4. Project Sustainable Mobility Centre (National Centre for Sustainable Mobility - CNMS) _Code CN000023, CUP: F83C22000720001" spoke 14. It was also supported by project RIPARTI(Ricerca Per riPARTire con le Imprese). POC PUGLIA FESR-fse 2014/2020.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.fuel.2024.132759>.

References

- [1] Zhang Y, Lu Q, Fan B, Long L, Quayle EK, Pan J. Effect of multiple bluff bodies on hydrogen/air combustion characteristics and thermal properties in micro combustor. *Int J Hydrogen Energy* Feb. 2023;48(10):4064–72. <https://doi.org/10.1016/j.ijhydene.2022.10.268>.
- [2] He Z, Zhang L, Li X, You J, Xue Z, Yan Y. Heat transfer enhancement and pressure loss analysis of hydrogen-fueled microcombustor with slinky projection shape channel for micro-thermophotovoltaic system. *Energy* Nov. 2023;283:129119. <https://doi.org/10.1016/j.energy.2023.129119>.
- [3] Hiranandani K, Aravind B, Ratna Kishore V, Kumar S. Development of a numerical model for performance prediction of an integrated microcombustor-thermoelectric power generator. *Energy* Feb. 2020;192:116624. <https://doi.org/10.1016/j.energy.2019.116624>.
- [4] Zuo W, Wang Z, Li Q, Zhou K, Huang Y. Numerical investigations on the performance enhancement of a hydrogen-fueled micro planar combustor with finned bluff body for thermophotovoltaic applications. *Energy* Apr. 2024;293:130752. <https://doi.org/10.1016/j.energy.2024.130752>.
- [5] Hyun Kim W, Seon Park T. Exploring combustion characteristics of a novel micro combustor with a fan swirler for thermophotovoltaic system. *Appl Therm Eng* May 2024;245:122795. <https://doi.org/10.1016/j.applthermaleng.2023.122795>.
- [6] Tohid F, Ghazanfari Holagh S, Chitsaz A. Thermoelectric Generators: A comprehensive review of characteristics and applications. *Appl Therm Eng* Jan. 2022;201:117793. <https://doi.org/10.1016/j.applthermaleng.2021.117793>.
- [7] Wang H, et al. Numerical investigation on thermal performance improvement of hydrogen-fueled tube with rib/fins for micro thermophotovoltaic. *Appl Therm Eng* Oct. 2023;233:121107. <https://doi.org/10.1016/j.applthermaleng.2023.121107>.
- [8] Yan Y, Zhang C, Gao J, Shen K, Gao W. Numerical study on premixed hydrogen/air combustion characteristics and heat transfer enhancement of micro-combustor embedded with pin fins. *Int J Hydrogen Energy* Nov. 2021;46(77):38519–34. <https://doi.org/10.1016/j.ijhydene.2021.09.097>.
- [9] Zuo W, et al. Effects of injection strategies on thermal performance of a novel micro planar combustor fueled by hydrogen. *Int J Hydrogen Energy* Feb. 2022;47(14):9018–29. <https://doi.org/10.1016/j.ijhydene.2021.12.206>.
- [10] Zhang C, et al. Study on synergistic heat transfer enhancement and adaptive control behavior of baffle under sudden change of inlet velocity in a micro combustor. *J Clean Prod* Jan. 2024;434:139856. <https://doi.org/10.1016/j.jclepro.2023.139856>.
- [11] Cai T, Zhao D, Karimi N. Optimizing thermal performance and exergy efficiency in hydrogen-fueled meso-combustors by applying a bluff-body. *J Clean Prod* Aug. 2021;311:127573. <https://doi.org/10.1016/j.jclepro.2021.127573>.
- [12] Li GY, Fan A. Non-premixed combustion characteristics and thermal performance of a catalytic combustor for micro-thermophotovoltaic systems. *Energy* Jan. 2021;214:118893. <https://doi.org/10.1016/j.energy.2020.118893>.
- [13] Ni S, Zhao D, You Y, Huang Y, Wang B, Su Y. NOx emission and energy conversion efficiency studies on ammonia-powered micro-combustor with ring-shaped ribs in fuel-rich combustion. *J Clean Prod* Oct. 2021;320:128901. <https://doi.org/10.1016/j.jclepro.2021.128901>.
- [14] Tang A, Zhang H, Cai T, Li C. Combustion and emission performance evaluation in ammonia/hydrogen-powered system with baffle and secondary injection applied. *Fuel* Jul. 2024;367:131457. <https://doi.org/10.1016/j.fuel.2024.131457>.
- [15] Ding J, J. E, Li J, Cai L, Luo B. Effect analysis on energy conversion enhancement of porous medium micro-combustor and thermoelectric system and its optimization. *Energy Convers Manage* Sep. 2023;292:117441. <https://doi.org/10.1016/j.enconman.2023.117441>.
- [16] Zuo H, Zhu Y, Wu S, Abubakar S, Li Y. Effect of a crossed-semicircular-plate on thermal performance of micro-combustor fueled by premixed hydrogen-air mixture. *Int J Hydrogen Energy* May 2022;47(39):17442–53. <https://doi.org/10.1016/j.ijhydene.2022.03.212>.
- [17] Alrebei OF, Le Page LM, McKay G, El-Naas MH, Amhamed AI. Recalibration of carbon-free NH₃/H₂ fuel blend process: Qatar's roadmap for blue ammonia. *Int J Hydrogen Energy* Jul. 2023;48(61):23716–36. <https://doi.org/10.1016/j.ijhydene.2023.03.045>.
- [18] Li J, J. E, Ding J, Cai L, Luo B. Numerical investigation of inserting conical ring into the micro-combustor with premixed hydrogen/air to enhance the heat transfer performance for the micro-thermophotovoltaic system. *Int J Hydrogen Energy* Jun. 2024;69:51–67. <https://doi.org/10.1016/j.ijhydene.2024.04.348>.
- [19] Kaisare NS, Vlachos DG. A review on microcombustion: Fundamentals, devices and applications. *Prog Energy Combust Sci* Jun. 2012;38(3):321–59. <https://doi.org/10.1016/j.pecs.2012.01.001>.
- [20] Zheng S, He Y, Liu H, Yang Y, Lu Q. Impacts of Radiation Reabsorption on the Flame Speed and NO Generation of CH₄/NH₃/Air Flames. *Energy Fuels* Apr. 2023;37(7):5632–43. <https://doi.org/10.1021/acs.energyfuels.3c00191>.
- [21] Newhall HK, Starkman ES. Theoretical Performance of Ammonia as a Gas Turbine Fuel. Warrendale, PA: SAE International; Feb. 1966. SAE Technical Paper 660768, doi: 10.4271/660768.
- [22] Li Z, Zhang Y, Zhang H. Kinetics modeling of NOx emission of oxygen-enriched and rich-lean-staged ammonia combustion under gas turbine conditions. *Fuel* Jan. 2024;355:129509. <https://doi.org/10.1016/j.fuel.2023.129509>.
- [23] Ariemma GB, Sorrentino G, Ragucci R, de Joannon M, Sabia P. Ammonia/Methane combustion: Stability and NOx emissions. *Combust Flame* Jul. 2022;241:112071. <https://doi.org/10.1016/j.combustflame.2022.112071>.
- [24] Zhu Z, et al. Experimental study on NOx reduction performance by ammonia solution injection into the fuel-rich zone in a 75 t/h coal-fired industrial boiler. *Fuel* Feb. 2024;357:129745. <https://doi.org/10.1016/j.fuel.2023.129745>.
- [25] Mehdi G, De Giorgi MG, Bonuso S, Shah ZA, Cinieri G, Ficarella A. Comparative Analysis of Flame Propagation and Flammability Limits of CH₄/H₂/Air Mixture with or without Nanosecond Plasma Discharges. *Aerospace* Feb. 2023;10:224. <https://doi.org/10.3390/aerospace10030224>.
- [26] Kobayashi H, Hayakawa A, Somaratne KDKA, Okafor EC. Science and technology of ammonia combustion. *Proc Combust Inst* Jan. 2019;37(1):109–33. <https://doi.org/10.1016/j.proci.2018.09.029>.
- [27] Lee JH, Kim JH, Park JH, Kwon OC. Studies on properties of laminar premixed hydrogen-added ammonia/air flames for hydrogen production. *Int J Hydrogen Energy* Feb. 2010;35(3):1054–64. <https://doi.org/10.1016/j.ijhydene.2009.11.071>.
- [28] Meng X, et al. Visualization and simulation study of ammonia blending with hydrogen as combustion application in lean-burn condition. *Fuel* Feb. 2024;357:129812. <https://doi.org/10.1016/j.fuel.2023.129812>.
- [29] Luo B, J. E, Chen J, Zhang F, Ding J. Effect of NH₃/H₂/O₂ premixed combustion on energy conversion enhancement and NOx emission reduction of the segmented nozzle micro-combustor in thermophotovoltaic system. *Renew Energy* Jul. 2024;228:120682. <https://doi.org/10.1016/j.renene.2024.120682>.
- [30] Han X, Wang Z, He Y, Zhu Y, Cen K. Experimental and kinetic modeling study of laminar burning velocities of NH₃/syngas/air premixed flames. *Combust Flame* Mar. 2020;213:1–13. <https://doi.org/10.1016/j.combustflame.2019.11.032>.
- [31] Zhang Y, Xiao S, Lu Q, Chen W, Quayle EK, Pan J. Numerical study on non-premixed combustion characteristics of NH₃/O₂ in multi-inlet micro combustor. *Appl Therm Eng* Apr. 2023;224:120091. <https://doi.org/10.1016/j.applthermaleng.2023.120091>.
- [32] You J, Wang D, Yan Y, He Z, Xue Z. A novel two-stage thermophotovoltaic-thermoelectric system based on micro combustion. *Appl Therm Eng* Sep. 2023;232:121018. <https://doi.org/10.1016/j.applthermaleng.2023.121018>.
- [33] Ilbas M. The effect of thermal radiation and radiation models on hydrogen-hydrocarbon combustion modelling. *Int J Hydrogen Energy* Aug. 2005;30(10):1113–26. <https://doi.org/10.1016/j.ijhydene.2004.10.009>.
- [34] S. Mazumder and S. P. Roy, 'Modeling Thermal Radiation in Combustion Environments: Progress and Challenges', *Energies*, vol. 16, no. 10, Art. no. 10, Jan. 2023, doi: 10.3390/en16104250.
- [35] A. shiblawi and A. Majhool, 'A comparative study of radiation models in spray combustion', *Al-Qadisiyah Journal for Engineering Sciences*, vol. 16, pp. 3–12, Mar. 2023, doi: 10.30772/qjes.v16i1.900.
- [36] N. Roberto Caetano, M. Schmitz Venturini, F. Roman Centeno, C. Katiushcia Lemmert, and K. G. Kyprianidis, 'Assessment of mathematical models for prediction of thermal radiation heat loss from laminar and turbulent jet non-premixed flames', *Thermal Science and Engineering Progress*, vol. 7, pp. 241–247, Sep. 2018, doi: 10.1016/j.tsep.2018.06.008.
- [37] Razmjooei B, Ravangard AR, Momayez L, Ferchichi M. The influence of heat transfer due to radiation heat transfer from a combustion chamber. *J Therm Anal Calorim* Feb. 2022;147(3):1901–17. <https://doi.org/10.1007/s10973-020-10263-3>.
- [38] Yang Z, Adeosun A, Kumfer BM, Axelbaum RL. An approach to estimating flame radiation in combustion chambers containing suspended-particles. *Fuel* Jul. 2017;199:420–9. <https://doi.org/10.1016/j.fuel.2017.02.083>.
- [39] M. V. N. Surendra Gupta et al., 'Numerical modeling and performance enhancement of micro combustor powered thermophotovoltaic systems using high contrast gratings', *Applied Thermal Engineering*, vol. 215, p. 118935, Oct. 2022, doi: 10.1016/j.applthermaleng.2022.118935.
- [40] I. S. Grigor'ev, 'Calculation of the absorption coefficient of air at different heights using the HITRAN and ACE-FTS databases', *J. Opt. Technol., JOT*, vol. 89, no. 10, pp. 578–585, Oct. 2022, doi: 10.1364/JOT.89.000578.
- [41] Z. Li et al., 'Research on Stellar Occultation Detection with Bandpass Filtering for Oxygen Density Retrieval', *Remote Sensing*, vol. 15, no. 14, Art. no. 14, Jan. 2023, doi: 10.3390/rs15143681.
- [42] Du Y, Li X, Shi L, Li F, Yuan S. Adaptive learning and expansion of spectral parameters in HITRAN database: A novel SCLB model for predicting high-temperature gas spectra. *J Quant Spectrosc Radiat Transf* Jan. 2024;313:108839. <https://doi.org/10.1016/j.jqsrt.2023.108839>.
- [43] Zheng S, Liu H, Li D, Liu Z, Zhou B, Lu Q. Effects of radiation reabsorption on the laminar burning velocity of methane/air and methane/hydrogen/air flames at elevated pressures. *Fuel* Mar. 2022;311:122586. <https://doi.org/10.1016/j.fuel.2021.122586>.
- [44] Liu H, Zheng S, He Y, Yang Y, Lu Q. Radiation effects of CO₂ and H₂O dilution on laminar flame speeds of syngas flames under elevated pressures. *Int J Hydrogen Energy* Dec. 2023;48(98):38870–7. <https://doi.org/10.1016/j.ijhydene.2023.06.189>.
- [45] Modest MF. In: 'Chapter 12 - Radiative Properties of Particulate Media', in *Radiative Heat Transfer (Third Edition)*. Boston: Academic Press; 2013. p. 387–439. <https://doi.org/10.1016/B978-0-12-386944-9.50012-1>.
- [46] CHMIELEWSKI, Maciej; GIERAS, Marian. Mean Absorption Coefficients of H₂O, CO₂, CO and NO for radiation numerical modeling in combustors flows. *Journal of Power Technologies*, [S.l.], v. 95, n. 2, p. 97–104, July 2015. ISSN 2083-4195.
- [47] Han L, Li J, Zhao D, Xi Y, Gu X, Wang N. Effect analysis on energy conversion enhancement and NOx emission reduction of ammonia/hydrogen fuelled wavy

- micro-combustor for micro-thermophotovoltaic application. *Fuel* Apr. 2021;289: 119755. <https://doi.org/10.1016/j.fuel.2020.119755>.
- [48] Mohammadpour A, Mazaheri K, Alipoor A, Mohammadpour M. Effect of oxidizer dilution on thermophotovoltaic performance of premixed ammonia/hydrogen/air combustion in radial micro-combustor. *Fuel* Jan. 2023;331:125874. <https://doi.org/10.1016/j.fuel.2022.125874>.
- [49] 'Ansys | Engineering Simulation Software'. Accessed: Jul. 20, 2023. [Online]. Available: <https://www.ansys.com/>.
- [50] Pannier E, Laux CO. RADIS: A nonequilibrium line-by-line radiative code for CO₂ and HITRAN-like database species. *J Quant Spectrosc Radiat Transf* Jan. 2019; 222–223:12–25. <https://doi.org/10.1016/j.jqsrt.2018.09.027>.
- [51] Wang A, Modest MF. Importance of Combined Lorentz-Doppler Broadening in High-Temperature Radiative Heat Transfer Applications. *J Heat Transfer Nov.* 2004;126(5):858–61. <https://doi.org/10.1115/1.1798951>.
- [52] Livadiotis G. Thermal Doppler Broadening of Spectral Emissions in Space and Astrophysical Plasmas. *ApJS* Dec. 2018;239(2):25. <https://doi.org/10.3847/1538-4365/aac835>.
- [53] I. Ventrillard, D. Romanini, D. Mondelain, and A. Campargue, 'Accurate measurements and temperature dependence of the water vapor self-continuum absorption in the 2.1 μm atmospheric window', *J Chem Phys*, vol. 143, no. 13, p. 134304, Oct. 2015, doi: 10.1063/1.4931811.
- [54] 'Infrared Region - an overview | ScienceDirect Topics'. Accessed: Feb. 02, 2024. [Online]. Available: <https://www.sciencedirect.com/topics/engineering/infrared-region>.
- [55] Mei B, et al. Experimental and kinetic modeling investigation on the laminar flame propagation of ammonia under oxygen enrichment and elevated pressure conditions. *Combust Flame* Dec. 2019;210:236–46. <https://doi.org/10.1016/j.combustflame.2019.08.033>.
- [56] Hashemi H, Christensen JM, Gersen S, Glarborg P. Hydrogen oxidation at high pressure and intermediate temperatures: Experiments and kinetic modeling. *Proc Combust Inst* Jan. 2015;35(1):553–60. <https://doi.org/10.1016/j.proci.2014.05.101>.
- [57] Shrestha KP, Seidel L, Zeuch T, Mauss F. Detailed Kinetic Mechanism for the Oxidation of Ammonia Including the Formation and Reduction of Nitrogen Oxides. *Energy Fuels* Oct. 2018;32(10):10202–17. <https://doi.org/10.1021/acs.energyfuels.8b01056>.
- [58] Konnov AA. On the role of excited species in hydrogen combustion. *Combust Flame* Oct. 2015;162(10):3755–72. <https://doi.org/10.1016/j.combustflame.2015.07.014>.
- [59] Chen X, Liu Q, Zhao W, Li R, Zhang Q, Mou Z. Experimental and chemical kinetic study on the flame propagation characteristics of ammonia/hydrogen/air mixtures. *Fuel* Feb. 2023;334:126509. <https://doi.org/10.1016/j.fuel.2022.126509>.
- [60] C. Lhuillier, P. Brequigny, N. Lamoureux, F. Contino, and C. Mounaïm-Rousselle, 'Experimental investigation on laminar burning velocities of ammonia/hydrogen/air mixtures at elevated temperatures', *Fuel*, p. 116653, Nov. 2019, doi: 10.1016/j.fuel.2019.116653.
- [61] Xiang Y, Wang S, Yuan Z, Fan A. Effects of channel length on propagation behaviors of non-premixed H₂-air flames in Y-shaped micro combustors. *Int J Hydrogen Energy* Aug. 2020;45(39):20449–57. <https://doi.org/10.1016/j.ijhydene.2019.11.147>.
- [62] Xiang Y, Yuan Z, Wang S, Fan A. Effects of flow rate and fuel/air ratio on propagation behaviors of diffusion H₂/air flames in a micro-combustor. *Energy* Jul. 2019;179:315–22. <https://doi.org/10.1016/j.energy.2019.05.052>.
- [63] Zhang C, et al. Numerical study on combustion characteristics and heat transfer enhancement of the micro combustor embedded with Y-shaped fin for micro thermo-photovoltaic system. *Appl Therm Eng* Jul. 2022;211:118427. <https://doi.org/10.1016/j.applthermaleng.2022.118427>.
- [64] Cinieri G, Shah ZA, Marseglia G, De Giorgi MG. Toward Zero Carbon Emissions: Investigating the Combustion Performance of Shaped Microcombustors Using H₂/Air and NH₃/Air Mixtures. *Aerospace* Dec. 2023;11(1):12. <https://doi.org/10.3390/aerospace11010012>.
- [65] G. Cinieri, D. Fontanarosa, and M. G. De Giorgi, 'Combustion Characteristics of Hydrogen/Air Mixtures in a Plasma-Assisted Micro Combustor', *Energies*, vol. 16, no. 5, Art. no. 5, Jan. 2023, doi: 10.3390/en16052272.
- [66] Nadimi E, Jafarmadar S. The numerical study of the energy and exergy efficiencies of the micro-combustor by the internal micro-fin for thermophotovoltaic systems. *J Clean Prod* Oct. 2019;235:394–403. <https://doi.org/10.1016/j.jclepro.2019.06.303>.
- [67] J. E et al., 'A comprehensive review on performance improvement of micro energy mechanical system: Heat transfer, micro combustion and energy conversion', *Energy*, vol. 239, p. 122509, Jan. 2022, doi: 10.1016/j.energy.2021.122509.
- [68] Ni S, et al. Thermal performances and emitter efficiency improvement studies on premixed micro-combustors with different geometric shapes for thermophotovoltaics applications. *Energy* Jul. 2021;226:120298. <https://doi.org/10.1016/j.energy.2021.120298>.
- [69] Bani S, Pan J, Tang A, Lu Q, Zhang Y. Numerical investigation of key parameters of the porous media combustion based Micro-Thermophotovoltaic system. *Energy* Aug. 2018;157:969–78. <https://doi.org/10.1016/j.energy.2018.05.151>.
- [70] Zuo W, J. E, W. Hu, Y. Jin, D. Han. Numerical investigations on combustion characteristics of H₂/air premixed combustion in a micro elliptical tube combustor. *Energy* May 2017;126:1–12. <https://doi.org/10.1016/j.energy.2017.03.011>.
- [71] Cai T, Zhao D. Effects of fuel composition and wall thermal conductivity on thermal and NO_x emission performances of an ammonia/hydrogen-oxygen micro-power system. *Fuel Process Technol* Dec. 2020;209:106527. <https://doi.org/10.1016/j.fuproc.2020.106527>.