

Research Paper

Numerical Study of Hydrogen Enrichment on Stoichiometric DME–Air Premixed Flames

Aris Purwanto¹, Herman Saputro², Akhmad Faruq Alhikami³, Riyadi Muslim⁴, Eka Dwi Ariyanto⁵, Fudhail Abdul Munir⁶

¹Department of Mechanical Engineering, Universitas Negeri Surabaya, Surabaya 60231, Indonesia

²Department of Mechanical Engineering Education, Universitas Sebelas Maret, Surakarta 57161, Indonesia

³Department of Mechanical Engineering, Universitas Islam Malang, Malang 65145, Indonesia

⁴Department of Mechanical Engineering, Universitas Sebelas Maret, Surakarta 57161, Indonesia

⁵Department of Mechanical Engineering, Universitas Negeri Surabaya, Surabaya 60231, Indonesia

⁶Faculty of Mechanical Engineering, Universiti Teknologi Petronas, Perak 31000, Malaysia

 arispurwanto@unesa.ac.id

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Abstract

Dimethyl ether (DME), an alternative fuel lacking carbon–carbon bonds, offers the potential for clean combustion with minimal soot emissions. Despite this advantage, DME exhibits relatively low initial reactivity and flame-propagation velocity under premixed conditions, which constrains its stability and operational flexibility. This study presents a numerical investigation of hydrogen enrichment effects on DME–air combustion characteristics and mechanisms, with emphasis on microkinetic behavior and flame structure. The investigation employs one-dimensional (1D) and two-dimensional (2D) simulations to assess adiabatic flame temperature, laminar flame propagation velocity, elementary reaction rates, dominant reaction pathways, and distributions of temperature and OH radicals. Results from 1D simulations indicate that introducing hydrogen at low fractions (approximately 5%) markedly increases both flame temperature and propagation velocity by enhancing the H–O–OH radical pool. When hydrogen fractions exceed 10%, further improvements in combustion performance plateau as the system nears chemical equilibrium. Kinetic analysis reveals that hydrogen acts as a key modulator, shifting DME oxidation from initiation-dominated reactions to hydrogen-abstraction and chain-branching regimes. Two-dimensional simulations corroborate that this mechanistic shift produces a more compact flame, advances heat release, and increases the concentration of OH radicals by an order of magnitude. Collectively, these results demonstrate that hydrogen functions as a microkinetic enhancer rather than merely a fuel additive and indicate that moderate enrichment (5–10%) is sufficient to optimize DME combustion.

Keywords: Dimethyl ether (DME); Hydrogen enrichment; Laminar flame speed; Combustion kinetics; Flame structure

1. Introduction

Technological advancements have facilitated the expansion of sectors such as transportation and industry. However, both sectors currently face a major challenge, namely the depletion of fossil fuel reserves in Indonesia [1]. In addition, fossil fuel combustion produces harmful emissions such as CO, CO₂, NO_x, and unburned

hydrocarbons (HC), which contribute to environmental pollution and global warming [2]. This condition demands the development of more sustainable, environmentally friendly energy solutions, primarily through the use of alternative fuels with cleaner, more efficient combustion characteristics.

In recent decades, researchers from various countries have developed and studied a range of



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environmentally friendly alternative fuels to reduce dependence on fossil fuels. Some alternative fuels that have been extensively researched include bio-based fuel [3], [4], ammonia [5], [6], [7], [8], and metal-based fuels [9], [10], [11], [12]. Various alternative fuels demonstrate significant potential to reduce emissions and decrease reliance on fossil fuels; however, each type encounters specific implementation challenges. Biodiesel and bioethanol, for instance, are constrained by limited raw material availability and competition with the food sector [13], [14]. Although ammonia is carbon-free, it has a low combustion rate and may generate elevated NO_x emissions [15], [16]. Furthermore, metal-based fuels require additional advancements in combustion processes and residue management technologies [17].

Dimethyl ether (DME) has attracted considerable attention as an alternative fuel due to its clean-burning characteristics. As an oxygenated fuel, DME can be produced from renewable sources such as biomass and carbon dioxide conversion, making it a promising candidate for sustainable energy systems [18], [19]. In addition, DME exhibits a high cetane number and favorable physical properties that enhance atomization and air–fuel mixing, enabling its application in various combustion systems. However, DME shows relatively low flame reactivity under lean conditions, which may affect flame stability and combustion performance [20], [21].

Hydrogen (H₂) has been extensively studied as a combustion enhancer to improve the performance of alternative fuels [22], [23], [24], [25], [26]. It exhibits advantageous combustion characteristics, such as low activation energy, high flame propagation speed, and high molecular diffusivity, which accelerate reaction kinetics and facilitate the formation of key radicals, including H and OH, that sustain flame propagation. Nevertheless, using hydrogen as a primary fuel introduces technical and safety challenges, such as flashback risks and storage difficulties. Consequently, enriching alternative fuels with small fractions of hydrogen is regarded as a more practical strategy.

Although hydrogen enrichment in DME combustion has been widely investigated, most previous studies varied equivalence ratio

simultaneously with hydrogen fraction, making it difficult to isolate the intrinsic kinetic effects of hydrogen addition [27], [28], [29]. Limited studies have systematically examined hydrogen-enriched DME–air flames under strictly stoichiometric conditions ($\phi = 1$). This study aims to numerically investigate the effect of hydrogen enrichment on the combustion characteristics of DME–air flames. In this work, simulations were performed using CHEMKIN-Pro and ANSYS Fluent to analyze several key combustion parameters, including laminar flame speed (LFS), adiabatic flame temperature (AFT), emission characteristics (NO, NO_x, and CO), reaction rate, reaction pathway, and two-dimensional flame structure. The results of the study are expected to provide a fundamental understanding of the role of hydrogen in DME–air combustion and to form the basis for the development of more efficient, low-emission combustion strategies.

2. Methods

A one-dimensional numerical simulation was performed using the CHEMKIN PRO software package [30], using the PREMIXED module to simulate laminar premixed flames [31]. This module solves the governing equations for mass, momentum, energy, and species conservation in a steady one-dimensional domain, enabling the investigation of fundamental flame characteristics under controlled conditions [32], [33]. The simulation produced detailed profiles of key parameters along the axial direction of the flame, such as temperature, velocity, pressure, and species concentrations. These results provide a validated kinetic baseline for reference. Additionally, the simulation facilitated analysis of reaction pathways by calculating reaction rates, species production and consumption rates, and the net heat release rate, all of which are critical for understanding flame structure and combustion behavior.

In numerical investigations of DME–H₂–air combustion, selecting an appropriate chemical kinetic mechanism is critical for ensuring both accuracy and computational efficiency. The present study utilizes a kinetic mechanism recently developed in the literature [34], which is specifically tailored for DME combustion systems and their mixtures with hydrogen. This mechanism was chosen because it accurately

captures the principal reaction pathways of DME and H_2 while involving fewer species and reactions than the Aramco mechanism. Unlike the highly detailed and computationally intensive Aramco mechanism, the selected mechanism is simpler and thus more suitable for parametric numerical simulations [35], [36]. Despite its reduced complexity, the mechanism retains the essential reactions governing the formation and consumption of major radicals such as H , O , and OH , as well as DME decomposition pathways that enhance flame reactivity through hydrogen enrichment. The mechanism accurately represents DME oxidation pathways and hydrogen-assisted radical chemistry; however, it does not explicitly include nitrogen chemistry or NO_x formation pathways. Therefore, to enable the prediction and analysis of NO_x emissions, a thermal NO sub-mechanism based on the Zeldovich formulation was manually incorporated into the original kinetic scheme [37]. The added reactions include $N_2 + O \rightleftharpoons NO + N$, $N + O_2 \rightleftharpoons NO + O$, and the extended Zeldovich reaction $N + OH \rightleftharpoons NO + H$, allowing NO_x formation to be dynamically coupled with local temperature and radical concentrations predicted by the H_2 -DME mechanism. This combined approach preserves the integrity of the original Wei *et al.* mechanism [34] while providing a physically consistent framework for evaluating NO_x emissions in hydrogen-enriched DME combustion systems.

Adaptive meshing was applied throughout the simulation to maintain stable and accurate numerical solutions. Mesh refinement was governed by two primary parameters: gradient-based control (GRAD) and curvature-based control (CURV), each with a sensitivity value of 0.1. The computational domain was limited to a maximum of 1000 grid points (NTOT), and 20 initial adaptive points were introduced to improve resolution in critical regions. The simulations included both thermal diffusion and multicomponent species transport to facilitate detailed modeling of flame dynamics. Mesh independence was evaluated by comparing temperature profiles generated with NTOT values of 1000 and 15,000. The results showed only minor discrepancies, indicating that further mesh refinement did not significantly influence the solution. Consequently, the simulation results

were considered grid-independent, demonstrating robustness with respect to spatial discretization.

A DME- H_2 -air mixture was used to investigate the effect of varying hydrogen fractions on premixed flame characteristics. Numerical simulations were conducted under ambient conditions, with an initial temperature of 300 K and a pressure of 1 atm. In addition to one-dimensional simulations, two-dimensional Computational Fluid Dynamics (CFD) simulations were performed to capture the spatial distribution of flow and reactive species. CFD software is commonly applied to combustion phenomena [38], [39], [40], [41], [42]. To minimize computational cost, a two-dimensional configuration was selected. ANSYS Fluent was used to analyze flame configuration and the spatial distribution of temperature and species within the burner geometry. Simulations were run on an Intel Core i7 computer with 16 GB of RAM. The SIMPLE algorithm with a pressure-based solver was applied. The governing equations included the steady-state two-dimensional Navier-Stokes equations together with conservation equations for mass, energy, and species transport [43]. The simulation was based on the following assumptions: (1) steady-state combustion, (2) Dufour and Soret effects neglected, (3) gas radiation neglected, (4) laminar flow, and (5) incompressible flow with ideal gas conditions. Based on these assumptions, the conservation equations are formulated as follows in Eq. (1) to Eq. (5).

Figure 1 illustrates the computational model used to investigate laminar premixed DME- H_2 -air flames with varying hydrogen enrichment levels. An open-domain configuration was adopted to capture flame development and eliminate artificial confinement effects that might alter flame structure and propagation. To improve computational efficiency and maintain numerical accuracy, the model exploited the flame's geometric symmetry by simulating only half of the computational domain. Dimethyl ether (DME) was selected as the primary fuel for its clean combustion characteristics, while hydrogen (H_2) was introduced as a secondary fuel to enhance flame reactivity. Hydrogen enrichment was systematically adjusted from 0 to 20% of the total fuel. The oxidizer was modeled as atmospheric air,

Continuity Conservation

$$\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial r} + \frac{\rho v}{r} = 0 \quad (1)$$

Momentum Equations

Axial Direction

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial r} = -\frac{\partial p}{\partial x} + \mu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\left(\frac{1}{r}\right) \partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right) \right) \quad (2)$$

Radial Direction

$$\rho u \frac{\partial v}{\partial x} + \rho v \frac{\partial v}{\partial r} = -\frac{\partial p}{\partial r} + \mu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\left(\frac{1}{r}\right) \partial}{\partial r} \left(r \frac{\partial v}{\partial r} \right) - \frac{v}{r^2} \right) \quad (3)$$

Energy Equation

$$\rho u \frac{\partial h}{\partial x} + \rho v \frac{\partial h}{\partial r} = \nabla \cdot (k \nabla T) + \sum h_i \dot{\omega}_i \quad (4)$$

Species Transport Equation

$$\rho u \frac{\partial Y_i}{\partial x} + \rho v \frac{\partial Y_i}{\partial r} = \nabla \cdot (\rho D_i \nabla Y_i) + \dot{\omega}_i \quad (5)$$

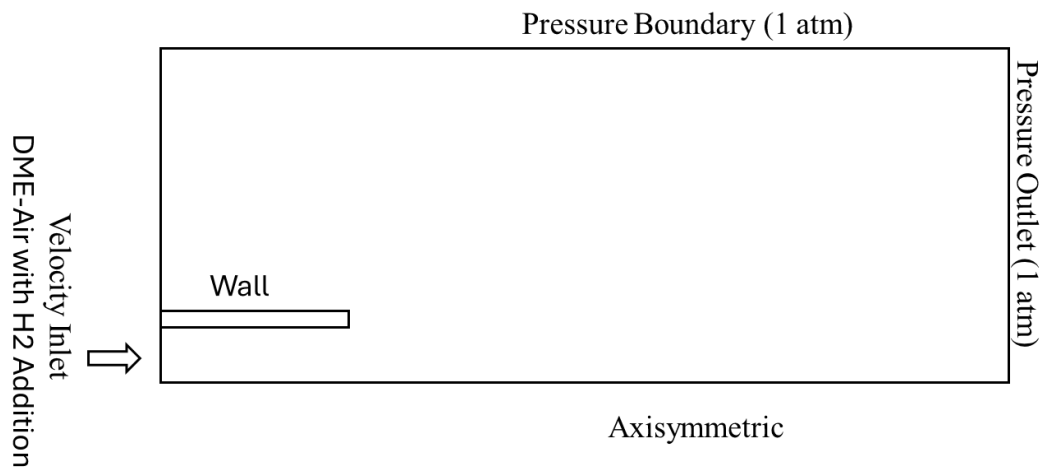


Figure 1. Computational domain

composed of 21% oxygen (O_2) and 79% nitrogen (N_2) by volume, as shown in Table 1. Before entering the computational domain, the fuel and oxidizer were assumed to be perfectly mixed, ensuring a fully premixed inlet for all simulations.

The flame was modeled as a laminar premixed flame, with the governing equations for mass, momentum, energy, and species transport solved using a laminar flow formulation. A turbulence model was not applied because the inlet velocity was low and there were no turbulence-generating mechanisms. This approach allows the resolution of intrinsic chemical kinetics and transport phenomena without uncertainties arising from

turbulence–chemistry interactions. Chemical reactions were described using a detailed kinetic mechanism for DME– H_2 –air combustion. The chemical source terms were directly coupled to the flow field, enabling accurate predictions of flame structure, temperature distribution, and species evolution. This modeling strategy provides a robust framework for evaluating the effects of hydrogen enrichment on laminar flame characteristics and the fundamental combustion behavior of DME–air mixtures. The computational domain was discretized using a tetrahedral mesh [44]. Mesh refinement was implemented, especially near the wall regions

Table 1. Mole fraction for each simulation case

H ₂ Addition (%)	DME Mole	H ₂ Mole	O ₂ Mole	N ₂ Mole
0%	0.0654	-	0.1963	0.7383
5%	0.0803	0.00423	0.2431	0.6724
10%	0.0794	0.00882	0.2425	0.6692
15%	0.0782	0.0138	0.2413	0.6667
20%	0.0769	0.0192	0.2404	0.6635

Table 2. Boundary conditions for 2D simulation

Boundary	Variable	Value
Inlet	Velocity Inlet	0.8 m/s
	Temperature	300 K
Outlet	Pressure Outlet	1 atm
	Mole Fraction	0.21 for O ₂ and 0.79 for N ₂
Equivalent Ration	Back-flow temperature	300 K
	ER	1
Wall	Wall Condition	No-Slip wall

adjacent to the reaction zone, to capture steep gradients in temperature and species concentration. To verify the numerical results' reliability, a grid independence test was performed by varying the mesh size. A refinement size of 0.2 mm produced the most stable flame-temperature results while also providing the lowest computational cost [43], [45]. Simulations were deemed converged when the residuals of the governing equations fell below 10^{-5} . This convergence criterion indicates that the iterative solution process achieved sufficient accuracy, as further iterations produced negligible changes.

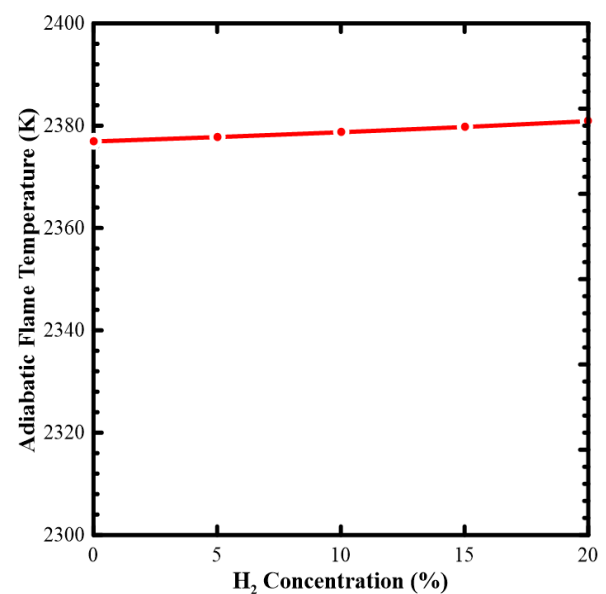
3. Results and Discussion

3.1. 1D Simulation

The first numerical simulation investigated the effect of H₂ addition on DME–air mixtures by evaluating the adiabatic flame temperature using CHEMKIN. The influence of hydrogen concentration on the adiabatic flame temperature (AFT) in stoichiometric premixed DME–H₂–air mixtures is shown in Figure 2. In the base DME–air flame, the AFT is recorded at 2376.9 K. The addition of 20% hydrogen results in a slight increase in AFT to 2380.88 K, indicating that hydrogen plays a substantial role in enhancing the reactivity of the fuel mixture. This marked increase is primarily due to elevated rates of radical reactions involving hydrogen atoms, such as $\text{H} + \text{O}_2 \rightarrow \text{OH} + \text{O}$ and $\text{OH} + \text{H}_2 \rightarrow \text{H} + \text{H}_2\text{O}$, which accelerate radical formation and raise flame temperature [46], [47]. This phenomenon suggests that although hydrogen exhibits a high reaction

rate, its contribution to increasing the adiabatic flame temperature becomes limited at higher hydrogen fractions because chemical equilibrium is attained under adiabatic conditions [48], [49].

These results indicate that adding a small amount of hydrogen is sufficient to effectively increase the flame temperature and combustion reactivity of DME–air mixtures. At the same time, additional additions provide diminishing thermal benefits. This finding is significant for the design of DME–H₂ combustion systems, as enhanced reactivity can be achieved without requiring high hydrogen fractions, thereby minimizing potential operational risks and system complexity. As a concrete design guideline, it is recommended that

**Figure 2.** Adiabatic flame temperature for different H₂ addition

the hydrogen fraction be maintained between 5% and 10%. This range ensures optimal improvements in combustion efficiency and flame temperature while avoiding the need for significant system redesigns. Such concentrations enable maximal utilization of hydrogen's potential without complications associated with higher ratios.

The laminar flame speed (LFS) in premixed DME–H₂–air mixtures is highly sensitive to hydrogen enrichment, as shown in Figure 3. In the absence of hydrogen, the LFS remains low at 46.2 cm/s, which reflects limited kinetic reactivity in DME–air combustion, particularly during flame propagation governed by active radical formation. The introduction of 5% hydrogen increases the LFS substantially to 73.8 cm/s. This enhancement indicates that even a small hydrogen fraction significantly accelerates key reaction pathways by increasing the concentrations of H and OH radicals. In the primary reaction $\text{H} + \text{O}_2 \rightarrow \text{OH} + \text{O}$, the higher reaction rate is evident in increased OH radical production. Subsequent reactions, such as $\text{O} + \text{H}_2 \rightarrow \text{OH} + \text{H}$ and $\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$, further demonstrate that minor H₂ additions elevate radical concentrations and markedly accelerate the overall reaction [50]. Therefore, low hydrogen fractions exert a dominant kinetic effect, resulting in the observed 60% increase in LFS. However, when the hydrogen fraction increases to 10–15%, the rise in LFS becomes more moderate, and at 20%, no further increase is observed. This behavior suggests a transition from a kinetically controlled to a transport-limited regime, in which heat and mass diffusion govern flame propagation. These results indicate that moderate hydrogen enrichment is sufficient to optimize laminar flame speed in DME–air flames.

The accuracy of the numerical results was evaluated by comparing the predicted laminar flame speeds with previously reported

experimental data [51]. The comparison shows good agreement, with deviations ranging from 2.56% to 7.31% across the investigated hydrogen fractions. Such deviations remain within an acceptable range for combustion simulations, indicating that the chemical kinetic mechanism employed in this study captures the fundamental flame-propagation characteristics of DME–H₂ mixtures.

Table 3 presents the effect of hydrogen addition on the laminar flame speed of DME–air mixtures at atmospheric pressure and an unburned temperature of 300 K. The results demonstrate a gradual increase in laminar flame speed with increasing hydrogen fraction. Specifically, the flame speed rises from 45.31 cm/s for pure DME to 48.20 cm/s at 20% H₂ addition, representing an enhancement of approximately 6.38%. This increase is attributed to the higher diffusivity of hydrogen and the enhanced production of reactive radicals such as H and OH, which accelerate overall combustion kinetics.

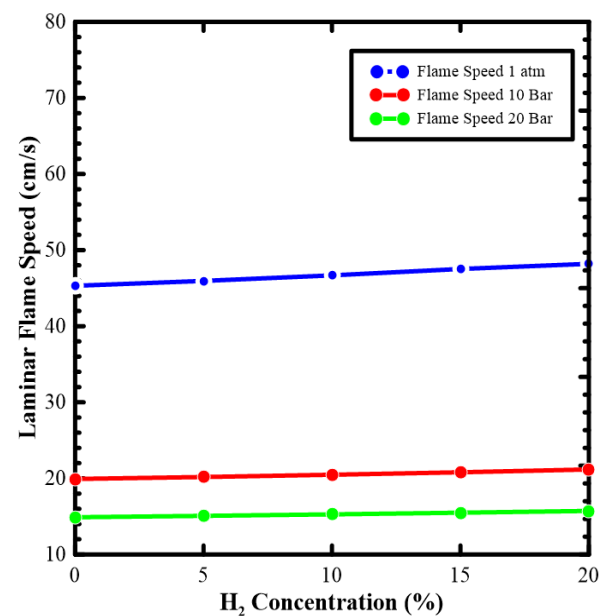


Figure 3. Laminar flame speed with different H₂ addition under elevated pressure

Table 3. Comparison of predicted laminar flame speeds with experimental data for DME–H₂–air mixtures at 1 atm and an initial temperature of 300 K

H ₂ Fraction (%)	Laminar Flame Speed (cm/s)	Experimental Data from Wang [51] (cm/s)	Deviation (%)
0	45.3	46.5	2.56
5	45.9	48	4.27
10	46.6	49.5	5.70
15	47.5	50.5	5.9
20	48.2	52	7.3

At elevated pressures representative of engine operation (10 and 20 bar), the laminar flame speed (LFS) decreases markedly compared to atmospheric conditions [29], [52]. At approximately 10 bar, LFS ranges from 19 to 21 cm/s, depending on hydrogen concentration. This reduction is primarily attributed to enhanced three-body recombination reactions, which decrease radical lifetimes and weaken chain-branching processes. At 20 bar, LFS further declines to 14 to 16 cm/s as recombination reactions become increasingly dominant and molecular diffusivity is further reduced. While hydrogen enrichment continues to increase LFS at high pressures, the magnitude of this enhancement diminishes. Consequently, moderate hydrogen addition (5 to 10%) mainly improves ignition stability and early flame development, rather than significantly increasing flame propagation speed.

The reaction $\text{CH}_3\text{OCH}_3 + \text{H} \rightleftharpoons \text{CH}_3\text{OCH}_2 + \text{H}_2$ constitutes a primary pathway by which hydrogen addition increases dimethyl ether (DME) flame reactivity, as illustrated in Figure 4. This process produces the CH_3OCH_2 radical, which facilitates subsequent oxidation reactions that yield formaldehyde and other intermediates. In the absence of hydrogen addition, the net reaction rate remains low ($\sim 10^{-5}$ mole/cm³.s) due to the limited availability of H radicals in pure DME-air flames [21]. When 20% hydrogen is introduced, the peak reaction rate rises by nearly an order of magnitude, and the reaction zone

becomes more concentrated, reflecting accelerated chemical kinetics [53]. The elevated H radical concentration intensifies hydrogen-abstraction reactions, thereby enhancing chain-propagation pathways and contributing to the observed increase in laminar flame speed in DME-H₂-air mixtures.

In the absence of hydrogen addition, the oxidation mechanism of dimethyl ether (DME) is primarily determined by the initial fuel cleavage pathway. As illustrated in Figure 5, the dominant reaction is $\text{CH}_3\text{OCH}_3 \rightarrow \text{CH}_3\text{O} + \text{CH}_3$, proceeding at a rate on the order of 10^{-6} . By comparison, the

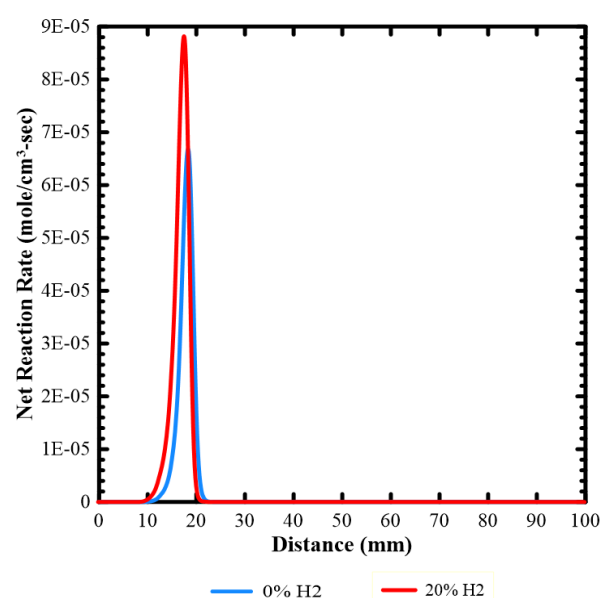


Figure 4. Net reaction rate of DME-air and DME-air with 20% H₂ addition

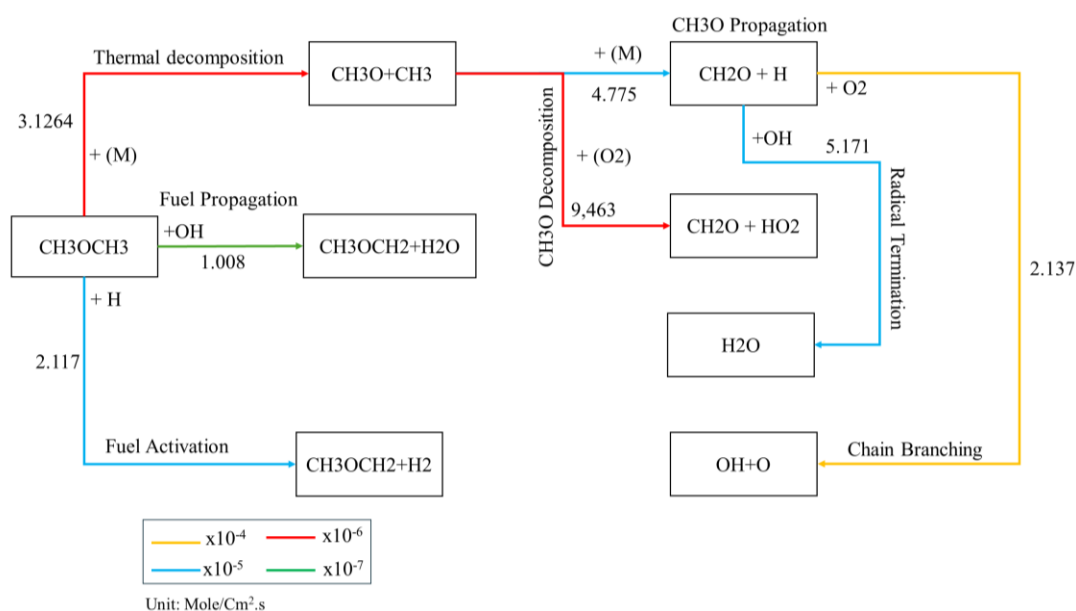


Figure 5. Reaction pathways for DME-air combustion

initiation step for methane under similar conditions (1 atm pressure, 298 K, and an equivalence ratio of 1.0) generally occurs at a higher order of magnitude, indicating that the overall initiation process for DME is slower [54]. Although this reaction constitutes the primary stage of radical formation, its relatively low intensity leads to slow propagation of subsequent reactions. As a result, the increase in flame temperature is limited. The hydrogen abstraction reaction from DME, $\text{CH}_3\text{OCH}_3 + \text{H} \rightarrow \text{CH}_3\text{OCH}_2 + \text{H}_2$, plays a secondary role, with reaction rates ranging from 10^{-5} to 10^{-7} . The low concentration of H radicals in pure DME–air flames restricts the formation of CH_3OCH_2 radicals, which are essential for accelerating subsequent oxidation pathways. Consequently, the reaction pathways leading to the formation of $\text{CH}_2\text{O} + \text{H}$ and $\text{CH}_2\text{O} + \text{HO}_2$ remain weak and are widely distributed throughout the reaction zone. Additionally, the limited production of OH and O radicals from formaldehyde conversion constrains the development of chain-branching reactions. These results indicate that the flame at 0% H_2 remains in a kinetic regime dominated by the initiation stage, resulting in a relatively low laminar flame speed for DME–air mixtures.

At a hydrogen enrichment level of 20%, the reaction mechanism shifts fundamentally. The hydrogen abstraction pathway, $\text{CH}_3\text{OCH}_3 + \text{H} \rightarrow \text{CH}_3\text{OCH}_2 + \text{H}_2$, illustrated in Figure 6, becomes the dominant route, with the reaction rate increasing to approximately 10^{-5} . This shift results from a substantial increase in the concentration of H radicals generated during hydrogen oxidation. Under these conditions, the formation of CH_3OCH_2 radicals is markedly accelerated, and these radicals serve as key intermediates in the dimethyl ether (DME) oxidation pathway. The CH_3OCH_2 radicals are rapidly converted to $\text{CH}_2\text{O} + \text{H}$ and $\text{CH}_2\text{O} + \text{HO}_2$, creating a more concentrated and localized reaction network within the flame zone. Furthermore, the reaction $\text{CH}_2\text{O} + \text{H} \rightarrow \text{OH} + \text{O}$ shows a significant rate increase, approaching 10^{-4} , indicating the onset of a chain-branching-dominated regime. The increased production of OH and O radicals further accelerates flame propagation and enhances flame stability [55], [56].

The increased formation of H_2O further demonstrates that exothermic reactions proceed

more rapidly and are concentrated near the flame front. This localized heat release intensifies the pressure–temperature gradient and strengthens the heat feedback mechanism within the flame. As a result, hydrogen enrichment promotes a more stable and efficient combustion process. In summary, hydrogen enrichment shifts the combustion mechanism from initiation-controlled kinetics to a regime dominated by hydrogen abstraction and chain-branching reactions. This mechanistic transition directly accounts for the significant increase in laminar flame speed and overall flame reactivity observed in DME– H_2 –air mixtures.

Nitric oxide (NO) formation in premixed DME– H_2 –air combustion is primarily controlled by the thermal NO (Zeldovich) mechanism, which is highly sensitive to flame temperature and the concentrations of reactive radicals. Figure 7 shows that the NO emission index (EINO) increases steadily with hydrogen addition from 0% to 20%, rising from approximately 6.85×10^3 to 7.05×10^3 g-NO/kg-fuel. The introduction of hydrogen increases the mixture's chemical reactivity, leading to higher flame temperatures and greater concentrations of key radicals, such as O, H, and OH, which, in turn, promote NO formation through extended Zeldovich reactions. Although EINO increases with hydrogen addition, the overall variation is moderate. This behavior is attributed to a slight reduction in nitrogen mole fraction as hydrogen replaces a portion of the base fuel. Consequently, while elevated temperatures and increased radical concentrations promote NO formation, the marginal decrease in nitrogen availability partially constrains the overall NO production rate. Furthermore, at hydrogen concentrations above approximately 10%, the flame temperature approaches a quasi-saturated regime, reducing the sensitivity of NO formation to further temperature increases. Under these conditions, the observed increase in EINO is primarily due to an enhanced radical pool, particularly OH radicals, which accelerate the $\text{N} + \text{OH} \rightarrow \text{NO} + \text{H}$ reaction along the extended Zeldovich pathway. Overall, these findings indicate that hydrogen enrichment leads to a slight but consistent increase in NO emissions, driven mainly by radical-enhanced nitrogen chemistry rather than by temperature effects alone.

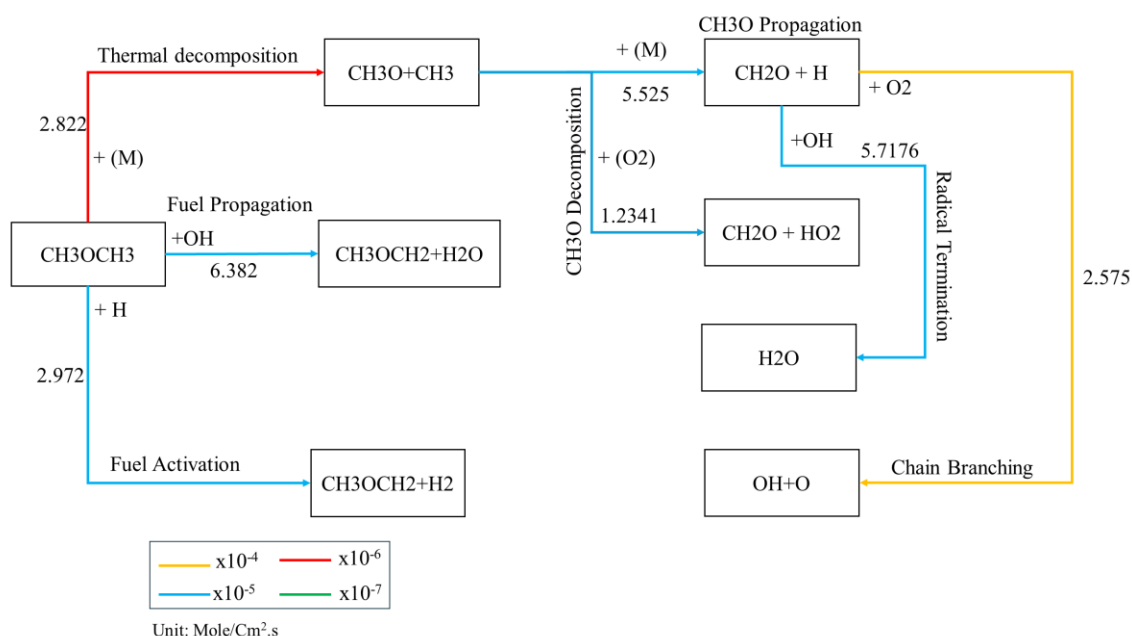


Figure 6. Reaction pathways for DME-air combustion with 20% H₂ addition

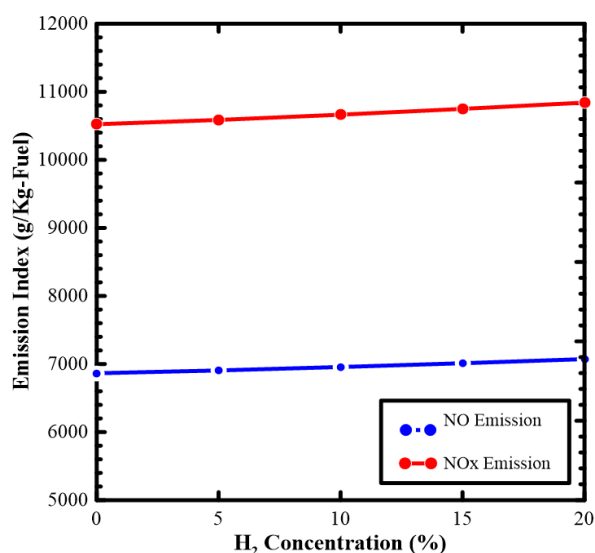


Figure 7. Variation of NO and NO_x emissions in premixed DME-H₂-air mixtures as a function of hydrogen concentration

3.2. 2D Simulation

The DME-air flame structure exhibits an elongated axial temperature distribution and a less localized high-temperature region. Temperature contours reveal a gradual increase from the pre-reaction zone to the flame core, which directly corresponds to the slower chain-branching rates inherent in the system's chemical kinetics, as shown in Figure 8. The upstream region maintains a minimum temperature of approximately 300 K, consistent with the inlet condition of the reactant mixture. The main

reaction zone is highly localized near the burner lip and displays a distinct temperature gradient from the blue to the red region. The peak temperature, approximately 2286 K, is consistent with the adiabatic flame temperature of stoichiometric DME-air without enrichment. This peak can be traced to specific elementary reaction steps, particularly the exothermic oxidation of DME to formaldehyde (CH₂O) and subsequent radical reactions. The CH₃OCH₂ + O₂ → CH₂O + CH₃O₂ pathway, for instance, plays a key role in driving the temperature toward its peak by influencing the overall heat release rate.

The temperature profile indicates that the heat release rate is concentrated in a thin reaction layer. This condition reflects the limitation of the initial reaction rate of DME, which is highly dependent on the hydrogen extraction process by OH and H radicals. According to research by Huang *et al.* [57], when hydrogen is not added to the DME-air mixture, there is no significant widening of the flame brush, indicating that thermal diffusivity and reactivity are predominantly controlled by the intrinsic properties of DME rather than the effects of fast diffusion observed with hydrogen. The OH mole fraction distribution supports this interpretation. According to Yu [53], The laminar flame speeds of DME mixtures decrease with increasing dilution ratio, reflecting changes in radical distribution and reaction dynamics within the flame. OH production mainly originates from

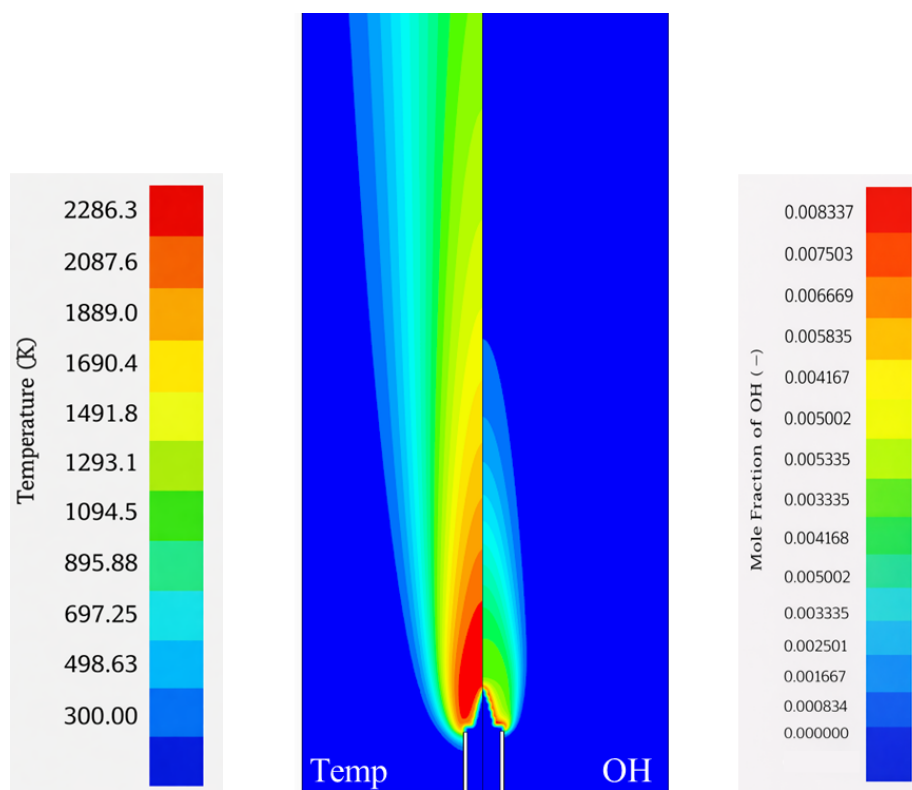


Figure 8. Flame temperature profile and OH radical of DME-air flame

the oxidation of formaldehyde (CH_2O) and the conventional pathway $\text{O} + \text{H}_2\text{O} \rightleftharpoons \text{OH} + \text{OH}$, both of which proceed with limited intensity in the absence of H_2 . This configuration indicates a kinetically controlled flame, characterized by a relatively low laminar flame speed and high sensitivity to reactant conditions.

The addition of 20% hydrogen leads to a substantial transformation in the DME–air flame structure, resulting in a more compact axial temperature profile and a more pronounced high-temperature region. Temperature contours indicate a rapid increase from the preheat zone to the flame core, which reflects accelerated chain-branching reactions facilitated by hydrogen enrichment. As in the base case, the upstream region maintains a minimum temperature of approximately 300 K, set by the inlet boundary condition (Table 2). Notably, the rapid temperature rise commences much closer to the burner lip, indicating earlier ignition and enhanced flame anchoring due to hydrogen's high diffusivity and reactivity, as shown in Figure 9. The peak temperature reaches approximately 2290 K, marginally higher than that of the pure DME–air flame, attributable to the enhanced heat release from hydrogen-assisted oxidation pathways.

The elevated temperature is primarily governed by rapid elementary reactions involving hydrogen radicals, particularly the $\text{H}-\text{O}-\text{OH}$ chain-branching loop, including $\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$ and $\text{O} + \text{H}_2 \rightarrow \text{H} + \text{OH}$. Given the high exothermicity of this reaction, the reverse step is significantly suppressed, which reassures that the forward direction proceeds essentially unidirectionally at flame temperatures. These reactions substantially increase the local concentration of OH radicals, which subsequently accelerate the oxidation of intermediate species produced from DME decomposition, such as formaldehyde (CH_2O) and methoxy radicals (CH_3O). Consequently, the heat release zone becomes thicker but shorter, indicating an increased laminar burning velocity and a reduction in the characteristic chemical time scale relative to the flow residence time.

The temperature profile also demonstrates that heat release is no longer restricted to a thin reaction layer, as observed in the pure DME case, but instead extends across a broader flame brush. This expansion results directly from hydrogen's high molecular diffusivity and low ignition energy, which enhance both thermal and mass transport within the flame. Unlike the kinetically

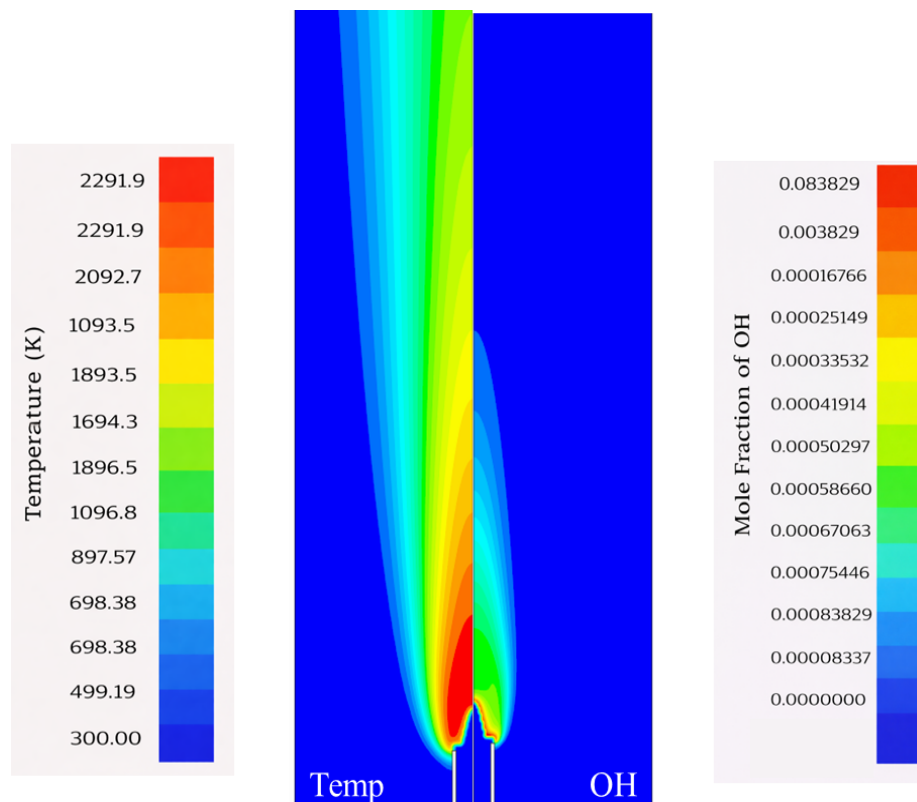


Figure 9. Flame temperature profile and OH radical of DME-air flame with 20% H₂ addition

limited behavior of pure DME combustion, the hydrogen-enriched flame operates in a reaction–diffusion coupled regime, where chemical kinetics and transport processes interact to intensify combustion.

The OH mole fraction distribution provides strong evidence for this interpretation. In comparison to the non-enriched case, the peak OH mole fraction increases by about one order of magnitude, and the OH-rich region expands significantly into the flame core. OH production is no longer dominated solely by formaldehyde oxidation and the conventional $O + H_2O \rightleftharpoons OH + OH$ pathway; instead, it is strongly driven by hydrogen-related reactions that maintain a high radical pool throughout the reaction zone. This elevated OH concentration promotes the oxidation of CO to CO₂ and stabilizes the flame under leaner or higher-strain conditions. As a result, the hydrogen-enriched DME flame exhibits a higher laminar flame speed, increased Damköhler number, and greater overall reactivity, although there is a potential for increased flashback susceptibility and thermal NO_x formation due to the higher temperature field.

4. Conclusion

Numerical simulations in one and two dimensions indicate that hydrogen addition significantly enhances the combustion characteristics of DME–air mixtures. A 5% H₂ addition significantly increases the adiabatic flame temperature and laminar flame speed due to enhanced formation of reactive radicals (H and OH). When H₂ fractions exceed 10%, further improvements are limited as the system approaches chemical equilibrium and becomes increasingly constrained by transport processes. Analysis of reaction rates and pathways shows that hydrogen enrichment increases the radical pool, shifting the DME oxidation mechanism from an initiation-controlled regime to one dominated by hydrogen-abstraction and chain-branching reactions. This mechanistic transition accounts for the increased flame propagation speed and reactivity observed in DME–H₂–air mixtures. Two-dimensional simulation results confirm distinct changes in flame structure with hydrogen addition, including a more compact temperature profile, earlier heat release, and an increase in both the concentration and spatial distribution of OH radicals by up to one order of magnitude.

Regarding emissions, NO and NO_x formation display a moderate increasing trend with higher hydrogen fractions. The enhancement of flame temperature and radical concentrations, particularly O and OH, promotes the thermal NO formation pathway via the extended Zeldovich mechanism. However, the increase in emission indices remains relatively limited, suggesting that hydrogen enrichment improves combustion performance without causing a disproportionate rise in nitrogen oxide emissions. Overall, these findings indicate that moderate hydrogen enrichment (5–10%) is sufficient to improve the stability, reactivity, and efficiency of DME combustion while maintaining relatively controlled NO and NO_x emissions. This provides a strong foundation for the development of efficient and cleaner DME–H₂ combustion systems. Future studies are recommended to further investigate the combustion characteristics of DME–H₂ mixtures at high pressure and across various equivalence ratios to better reflect practical operating conditions in gas turbine combustion systems.

Author's Declaration

Authors' contributions and responsibilities

The authors made substantial contributions to the conception and design of the study. The authors were responsible for data analysis, interpretation, and discussion of the results. The authors read and approved the final manuscript.

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