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A numerical study on premixed laminar ammonia/air flames enriched with hydrogen: An analysis on flame–wall interaction

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ABSTRACT

Ammonia (NH₃) has been recognized as a potential carbon-free synthetic fuel of the near future. To enhance its low reactivity, one practical option is to blend it with hydrogen (H₂). In this study, the transient head-on quenching of premixed laminar ammonia/air flames enriched with hydrogen is explored based on numerical simulations using detailed chemistry and the mixture-averaged transport model. In this respect, nine different test cases are studied for blending ratios (the molar ratio of hydrogen to the ammonia/hydrogen mixture) of 0.0, 0.2, and 0.4, equivalence ratios of 0.8, 1.0, and 1.2, wall temperatures of 300, 500, and 750 K, and pressures of 1, 2, and 5 atm. The results reveal that the quenching distance (maximum absolute wall heat flux) decreases (increases) with increasing the blending ratio, the equivalence ratio, the wall temperature, and the pressure. For all the test cases, the quenching Peclet number changes between 1 and 3.5. In addition, the local heat release rate enhancement and the role of radical recombination reactions are highlighted at the time of quenching in the vicinity of the wall. This effect is augmented as the blending ratio, the equivalence ratio, and the wall temperature increase. Furthermore, the results show that the N₂ pathway is the dominant pathway in consumption of NO near the wall at the time of quenching, in which R76 (NH + NO ⇌ N₂ + H₂O) poses the rate controlling role. In addition, the leading role of R85 (NH + NO ⇌ N₂O + H) in consuming NO and converting it to N₂O is highlighted at the time of quenching near the wall. Moreover, the significant roles of molecular diffusion and reaction source terms over convection are discussed for both NO and N₂O species transport in the vicinity of the wall.

Novelty and significance statement: The significance of this work is that using ammonia and its blends with hydrogen as promising carbon-free fuels for the future has several technical issues/uncertainties, which needs to be addressed fundamentally. One of the relatively unexplored issues in the combustion devices for ammonia/hydrogen/air flames is the head-on quenching phenomenon, which is investigated in detail in this study. The novelty of this work is that, for the first time, (1) the head-on quenching of various ammonia/hydrogen blends is systematically studied numerically, employing detailed chemistry, (2) effect of wall on the heat release rate chemistry is discussed wherein the role of radical recombination reactions is highlighted, and (3) the formation pathways of pollutant emissions (NO and N₂O) for such flames are thoroughly investigated in the freely propagating flame scenario and in the vicinity of the wall at the time of quenching.

1. Introduction

The dominant energy conversion methods for civil and industrial applications have relied on combustion processes, which are still heavily dependent on hydrocarbon fuels [1,2]. However, finite sources of fossil fuels, climate change, and environmental pollution result in the swift development of cutting-edge combustion technologies for transportation, marine sector, power generation, and industrial processes [3,4]. The key targets of these combustion technologies are to increase the system efficiency, decrease the pollutant emissions, and enhance load and fuel flexibility [3]. It is important to note that by utilizing carbon-free fuels such as ammonia (NH₃) for power generation and industrial processes, the targets for low carbon dioxide emissions could be achieved [1]. However, the low laminar burning velocity and heat of combustion of NH₃/air flames are obstacles in utilizing it smoothly in combustion processes. Thus, enhancing the combustion properties.
of ammonia is required in order to make it a viable fuel. In this regard, adding hydrogen (H₂) to ammonia is a practical approach to enhance its combustion characteristics [1]. However, the level of NOx emissions increases significantly by enriching it with hydrogen [5,6]. It should be noted that despite the extensive and ongoing research in utilizing ammonia as a fuel in combustion processes, see e.g. the review papers by Valera-Medina et al. [7], Kobayashi et al. [1], Dimitriou and Javaid [4], and Elbaz et al. [2], there still exist many unresolved problems regarding the utilization of such fuel in practical combustion devices.

One of the issues that is required to be addressed for NH₃/air flames is their interaction with walls. This phenomenon, flame–wall interaction (FWI), exists in the majority of combustion devices, resulting in several effects on the overall efficiency of the system, the formation of pollutants, and the lifetime of the combustion devices [8]. It should be emphasized that flames approaching the wall do not typically touch it; they quench a few micrometers away from the wall, since the wall with low temperature is capable of suppressing the chemical reactions [8]. Furthermore, the wall experiences high wall heat flux values for a short duration throughout the quenching process due to the existence of a large temperature gradient in the close proximity of the wall [8,9].

According to the review paper by Dreizler and Böhm [3], wall quenching can be classified into two extreme conditions of head-on quenching (HOQ) and side-wall quenching (SWQ). In the former, the flame propagates perpendicular to the wall, while in the latter, the flame propagates parallel to the wall. Generally, the quenching distance, which is defined as the minimum distance between the flame and the wall, is divided by the diffusive flame thickness, defined as the ratio of the thermal diffusivity to the unstrained premixed laminar burning velocity, to form a non-dimensional number, which is known as the quenching Peclet number (PeQ) [10,11]. This number essentially helps to compare the quenching distances for various fuels under different mixture compositions [12]. By examining the quenching Peclet numbers reported in the literature, Dreizler and Böhm [3] mentioned that this number falls within the range of 3.5±1 for head-on quenching, and it is essentially independent of the equivalence ratio and the fuel type, with the exception of hydrogen. However, this number is approximately 7 for side-wall quenching [8]. Furthermore, the wall heat flux varies with time during FWI, and it reaches its maximum value during the quenching process, see e.g. Huang et al. [11], Poinset et al. [9], Hasse et al. [13], Boust et al. [14], Owston et al. [15], Salimath et al. [16], and Zirwes et al. [12]. The quenching distance and the maximum wall heat flux depend on the wall temperature [13,17], the pressure [13–15,18–20], the reactants temperature [18], the equivalence ratio [14,18,20], and the fuel type [12,20].

It is important to note that gas-phase radical recombination reactions, which are identified by low-activation energy (or zero-activation energy [21]) reactions, play an important role during the quenching process. Therefore, using a single-step chemistry does not provide accurate results for this process [21]. The importance of these recombination reactions during the quenching process has already been discussed for hydrocarbon flames, see e.g. Westbrook et al. [22], Hocks et al. [23], Ezekoye et al. [24], Popp et al. [25], Popp and Baum [17], and Palulli et al. [26], and for hydrogen flames, see e.g. Owston et al. [15], Gruber et al. [21], and Salimath et al. [27].

It should be emphasized that exploring the formation of nitric oxide (NO) and nitrous oxide (N₂O) near the wall during flame–wall interaction is of great interest due to the environmental concerns regarding these species, especially for ammonia flames. Such exploration requires some understanding of the ammonia oxidation and NOx chemistry. Ammonia oxidation chemistry has been studied extensively for the last few decades, see e.g. Miller and Bowman [28] and Glarborg et al. [29], due to its fuel NOx formation and its utilization as a reducing agent in selective non-catalytic reduction of NOx [30], Kobayashi et al. [1] and Elbaz et al. [2] reviewed the ammonia oxidation chemistry and NOx chemistry of lean and rich ammonia flames. Lindstedt et al. [31] showed that NO is primarily produced through the nitrosyl (HNO) pathway for a set of laminar ammonia-blended flames. Recently, Karimkashi et al. [6] showed the importance of HNO and N₂O pathways for freely propagating laminar and turbulent ammonia flames enriched with hydrogen. Wang et al. [32] showed the effects of the equivalence ratio and hydrogen content in ammonia/hydrogen mixtures on NO, N₂O, and NO₂ levels for laminar flames under engine-relevant conditions. It should be highlighted that, regarding the existing literature in the community, there is no systematic and comprehensive study discussing the formation of pollutant emissions, i.e. NO and N₂O, in the vicinity of the wall during the interaction between ammonia-blends (flames) and the wall.

To the best of the authors’ knowledge, the quenching distance, the wall heat flux, the heat release rate chemistry, as well as the formation of pollutant emissions of NH₃/air and NH₃/H₂/air flames during the head-on quenching process are not thoroughly addressed in the literature. Understanding these details helps to explore the underlying physics behind such flames, and the results could further be utilized for developing combustion models near the wall and for designing state-of-the-art combustion devices. Therefore, the current study aims to examine these properties based on numerical simulations using detailed chemistry and the mixture-averaged transport model. In this regard, the main objectives of the present work are (1) to study the quenching distance and the wall heat flux, (2) to analyze the heat release rate variation, and to detect the contribution of the important chemical reactions to the heat release rate near the wall, and (3) to investigate the formation of pollutant emissions for ammonia-blended flames under various operating conditions during flame–wall interaction. The remainder of this paper is organized as follows. The computational methodology is discussed in Section 2. The validation test cases are described in Section 3. This is followed by Section 4 discussing the results of the current work. Finally, the concluding remarks are outlined in Section 5.

2. Computational methodology

In this section, a detailed description of the reactive flow solver, followed by the computational setup as well as the boundary conditions utilized in the current study is given.

2.1. Reactive flow solver

The open-source C++ CFD toolbox OpenFOAM-v8 [33,34] is utilized to solve the mass, momentum, species mass fractions, and energy conservation equations using the PIMPLE algorithm. In this study, detailed chemistry and the mixture-averaged transport model are used to accurately simulate the head-on quenching process of premixed laminar NH₃/air flames enriched with H₂.

The chemical kinetic mechanism developed by Stagni et al. [35] is used in the current study. This mechanism has 31 species and 203 reactions. The performance of this mechanism over a wide range of experimental conditions is reported by Shrestha et al. [36]. Recently, Lhuillier et al. [37] measured the laminar burning velocity of NH₃/H₂/air flames under various test conditions. Table 1 shows a concise comparison between the laminar burning velocity data obtained from freely propagating premixed flame simulations using Cantera [38] with the Stagni chemical kinetic mechanism and the available experimental data acquired from Lhuillier et al. [37] (relatively high reactants temperature) and Gotama et al. [39] (high reactants pressure). These data indicate that selecting the Stagni chemical kinetic mechanism is justifiable in the current study due to its satisfactory performance at relatively high reactants temperature and pressure. It should be borne in mind that the test cases studied in this work are at different operating conditions, which will be introduced later.

Gotama et al. [39] optimized and built a reduced chemical kinetic mechanism from the existing mechanism proposed by Han et al. [40].
This mechanism, which contains 26 species and 119 reactions, is capable of capturing the aforementioned experimental data on the laminar burning velocity competently. As a result, a sensitivity analysis is performed on the quantitative values of quenching distance and maximum absolute wall heat flux using Gotama et al. [39] and Stagni et al. [35] mechanisms, as shown in Figs. A.1 and A.2 in the supplementary material, to find out how the choice of different chemical kinetic mechanisms affects important parameters in the head-on quenching process. In this study, the instantaneous wall heat flux ($\phi_w$) is evaluated as $\phi_w = -\lambda \frac{\partial T}{\partial x_w}$, where $\lambda$ is the gas-phase thermal conductivity, $T$ is the temperature, the $x$ axis is considered normal to the wall, and $W$ represents the quantities at the wall [6].

The reactingDNS solver is utilized in this study. The successful implementation of this solver for reactive flow simulations has been shown earlier in several studies, see e.g. Refs. [6,41–46]. This solver is capable of using the mixture-averaged transport model for describing the reaction-diffusion process accurately. It should be emphasized that using this transport model leads to more accurate results compared to the models using unity/non-unity Lewis number assumption, specially for mixtures having high mass diffusivity species such as molecular hydrogen. In the current study, a second-order implicit backward Euler method and cubic interpolation scheme have been utilized for time and spatial discretizations, respectively. The reader is referred to Zirwes et al. [47,48] for more information on the cubic discretization scheme implemented in OpenFOAM.

The viscosity and thermal conductivity for each species as well as the binary diffusion coefficient for each species pair are estimated using third-order logarithmic polynomial fits based on the Chapman–Enskog solution of the Boltzmann equation. For evaluating the viscosity of the mixture, the Wilke mixing formula [49] is utilized herein. Furthermore, a combination averaging formula is used for calculating the mixture-averaged thermal conductivity [50]. For evaluating the mixture-averaged diffusion coefficient for each species, the methodology described by Bird et al. [51] is utilized. The thermodynamic properties of each species are evaluated from the polynomials fitted to JANAF-NIST thermochemical tables. These data are then used to estimate the thermodynamic properties of the mixture. It should be noted that the thermal diffusion effect (Soret effect) is neglected in the current study. Gruber [52] discussed that the flame–wall interaction process seems to be qualitatively unaffected by either including or excluding the Soret effect. He showed that neglecting the Soret effect from the head-on quenching simulations of premixed laminar hydrogen/air flames results in increasing the wall heat flux by about 10%, and decreasing the quenching distance by 5%–10%. Furthermore, Yu et al. [20] very recently demonstrated that this effect plays a minor role in the quenching distance values of pure ammonia/air flames, whereas its influence is enhanced by enriching the mixture with hydrogen. However, the role of Soret diffusion on one of the test conditions examined in this work is explored, and its results are provided in the supplementary material (see Fig. B.1).

To overcome the computational load imbalance among the parallel tasks, an open-source dynamic load balancing model (DLBFoam) developed by Tekgül et al. [53] is used. This model distributes the computation of chemistry problems equally among all the processors using the MPI communication protocol. This model has been used in several studies in the past, see e.g. [6,54–57].

The open-source library pyJac [58] is implemented within DLBFoam, which is herein linked to the reactingDNS solver. This library, which provides C subroutines, generates the analytical Jacobian of a prescribed chemical kinetic mechanism. The analytical Jacobian is required for solving a system of ordinary differential equations (ODE) to estimate the chemical source terms such as the heat release rate in the energy equation and the net consumption/production rate of each species in the species transport equations. The state of each computational cell is defined by pressure, temperature, and species mass fractions, i.e. the local thermochemical composition vector. It should be noted that the chemical source terms introduce high stiffness to the system of ordinary differential equations since the chemical time scales are much smaller than the flow time scale. Thus, an operator-splitting approach is used in order to separate the calculation of the chemistry problem from the fluid flow solution. These source terms, which represent the rate of change of the local thermochemical composition, are calculated by solving the system of ODEs using semi-explicit Euler method (Seulex) through integrating in each computational chemistry problem over the CFD time step [59].

### 2.2. Computational setup, boundary conditions, and test cases

In the current study, each test case is composed of 11,200 cells distributed evenly in a 1-D domain of 2.24 cm. This results in having a cell size of 2 μm for all the test conditions. It should be noted that a thorough grid independence study is carried out to determine this cell size, and the results are presented in Fig. C.1 in the supplementary material. In this 1-D computational domain, the solid wall is assigned to be on the left hand side of the domain, while the right hand side corresponds to the outlet boundary. The schematic representation of the computational domain is shown in Fig. 1.

As initial condition, the solution of a 1-D freely propagating flame obtained from Cantera is mapped on the computational domain, and the fluid flow velocities are set to zero across the domain. It should be emphasized that the flame profile is initiated far away from the wall ensuring that the wall does not have any initial effect on it. The species boundary condition is set to zero gradient for both the outlet and wall regions. The temperature boundary condition is a fixed temperature at the wall, which is equal to the reactants temperature for all the test conditions, and it is a zero gradient at the outlet region. For pressure, a non-reflecting and a zero gradient boundary conditions are applied to the outlet and the wall, respectively.

In this study, nine different test cases are primarily simulated exploring the effects of the blending ratio ($\alpha$), the equivalence ratio ($\phi$), the wall temperature ($T_w$), and the pressure ($P$) during the head-on quenching process. The blending ratio is the molar ratio of hydrogen to the ammonia/hydrogen mixture. Basically, the blending ratio varies from 0 (pure ammonia/air flame) to 0.4, and the equivalence ratio changes from 0.8 (lean condition) to 1.2 (rich condition). In addition, the wall temperature ranges from 300 to 750 K, and the pressure changes from 1 to 5 atm. According to Popp et al. [25], when the temperature of solid surfaces exceeds 400 K, depending on their material types, they have the potential to behave as catalysts. As a result, they can affect the flame–wall interaction phenomena. However, in the current study, following the approach of Gruber et al. [21], the wall surface chemistry is excluded from numerical simulations in order to avoid introducing wall material details as an additional parameter.

### Table 1

<table>
<thead>
<tr>
<th>$\alpha$ (-)</th>
<th>$\phi$ (-)</th>
<th>$T_w$ (K)</th>
<th>$P$ (atm)</th>
<th>$S_0^L$ (cm/s)</th>
<th>$S_0^H$ (cm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.0</td>
<td>473</td>
<td>1.0</td>
<td>17.53</td>
<td>16.08</td>
</tr>
<tr>
<td>0.2</td>
<td>0.4</td>
<td>473</td>
<td>1.0</td>
<td>31.96</td>
<td>32.23</td>
</tr>
<tr>
<td>0.4</td>
<td>0.8</td>
<td>473</td>
<td>1.0</td>
<td>69.83</td>
<td>67.10</td>
</tr>
<tr>
<td>0.0</td>
<td>1.2</td>
<td>473</td>
<td>1.0</td>
<td>52.85</td>
<td>53.34</td>
</tr>
<tr>
<td>0.0</td>
<td>1.0</td>
<td>298</td>
<td>5.0</td>
<td>66.16</td>
<td>69.07</td>
</tr>
<tr>
<td>0.4</td>
<td>1.0</td>
<td>298</td>
<td>5.0</td>
<td>15.46</td>
<td>14.41</td>
</tr>
</tbody>
</table>
methane/air flame reported earlier in [12], and the second one is a fuel cases. The first validation case is a stoichiometric premixed laminar in order to tackle this problem is validated using two different single nia/hydrogen flames in the context of head-on quenching that could there are no experimental results available using ammonia or ammo-

terature, respectively.

The results show that the maximum absolute wall heat flux values are along with the wall heat flux values reported by Owston et al. [15]. This observation is in line with the quenching Peclet number values reported earlier by Zirwes et al. [12] for the same test case, simulated with the EBiDNSFoam solver [47,48]. They mentioned that the quenching Peclet number values vary from 2.6 to 2.9 using 20 different chemical kinetic mechanisms available in the literature, including the GRI 3.0 chemical kinetic mechanism.

For the hydrogen/air flame validation test case, a computational domain of 2.24 cm containing 5600 cells (cell size of 2 μm) is utilized to estimate the quenching distance and the maximum absolute wall heat flux. The reactants and wall temperatures are set to 750 K and the pressure is fixed at 1 atm. It should be noted that the exact chemical kinetic mechanism used in the validation test case reported by Owston et al. [15] could not be found. As a result, three different chemical kinetic mechanisms, widely used for hydrogen flames, are utilized to assess the aforementioned parameters, namely, the mechanisms developed in Li et al. [65], Ő Conaire et al. [66], and Konnov [67].

Fig. 2 shows the transient absolute wall heat flux profiles for this test condition using the aforementioned chemical kinetic mechanisms along with the wall heat flux values reported by Owston et al. [15]. The results show that the maximum absolute wall heat flux values are equal to 2.90, 2.98, and 3.26 MW/m² using Li, Ő Conaire, and Konnov chemical kinetic mechanisms, respectively. This observation shows that the reported maximum absolute wall heat flux values, especially those evaluated with the Li and Ő Conaire chemical kinetic mechanisms, are in reasonable agreement with the value of 2.65 MW/m² reported earlier by Owston et al. [15]. Furthermore, the flame position is defined as the location where the iso-contour of temperature is equal to 1500 K, similar to Owston et al. [15]. This results in the quenching distances of 58, 52, and 54 μm using Li, Ő Conaire, and Konnov mechanisms, respectively. The obtained data are about 19–28% lower than the quenching distance value of 72 μm, which is reported earlier by Owston et al. [15]. It should be noted that the cell size used by Owston et al. [15] in their

Therefore, the analysis performed herein is not restricted to a partic-

ular wall material. As a result, the wall is assumed to be inert. This assumption has been utilized earlier in several studies, see e.g. Hasse et al. [13], Gruber et al. [21], Palulli et al. [26], Jiang et al. [60], and Salimath et al. [16]. It should be noted that in the flame–wall interaction studies, the radiative heat fluxes are generally disregarded due to their small values compared to the maximum heat flux acquired when the flame interacts with the wall [8]. Therefore, the radiative heat transfer is neglected in the current study. This assumption is inline with previous works in the literature, see e.g. [11,16,21,24–27]. These studies utilized different fuels in their numerical simulations, ranging from methane, propane, ethylene, to hydrogen. Furthermore, the radiative heat flux was modeled in Stagni et al. [61] for premixed laminar dimethyl ether (DME) flames. In their study, the radiative heat flux was found to have a negligible impact on their flame–wall interaction results [62]. Very recently, Steinhausen et al. [63] quantified the minor effect of radiative heat transfer on their results for side-wall quenching of partially premixed laminar methane/air flames. Table 2 summarizes the test conditions studied in this work in detail.

### Table 2

<table>
<thead>
<tr>
<th>Case</th>
<th>α (-)</th>
<th>φ (-)</th>
<th>T₀ (K)</th>
<th>P (atm)</th>
<th>S₀ (cm/s)</th>
<th>δ₀ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0</td>
<td>1.0</td>
<td>500</td>
<td>1.0</td>
<td>19.43</td>
<td>1.320</td>
</tr>
<tr>
<td>2</td>
<td>0.2</td>
<td>1.0</td>
<td>500</td>
<td>1.0</td>
<td>35.93</td>
<td>0.812</td>
</tr>
<tr>
<td>3</td>
<td>0.4</td>
<td>1.0</td>
<td>500</td>
<td>1.0</td>
<td>78.32</td>
<td>0.460</td>
</tr>
<tr>
<td>4</td>
<td>0.4</td>
<td>0.8</td>
<td>500</td>
<td>1.0</td>
<td>60.70</td>
<td>0.507</td>
</tr>
<tr>
<td>5</td>
<td>0.4</td>
<td>1.2</td>
<td>500</td>
<td>1.0</td>
<td>72.83</td>
<td>0.508</td>
</tr>
<tr>
<td>6</td>
<td>0.4</td>
<td>1.0</td>
<td>300</td>
<td>1.0</td>
<td>31.08</td>
<td>0.586</td>
</tr>
<tr>
<td>7</td>
<td>0.4</td>
<td>1.0</td>
<td>750</td>
<td>1.0</td>
<td>186.19</td>
<td>0.362</td>
</tr>
<tr>
<td>8</td>
<td>0.4</td>
<td>1.0</td>
<td>500</td>
<td>2.0</td>
<td>63.35</td>
<td>0.273</td>
</tr>
<tr>
<td>9</td>
<td>0.4</td>
<td>1.0</td>
<td>500</td>
<td>5.0</td>
<td>44.25</td>
<td>0.147</td>
</tr>
</tbody>
</table>

For the methane/air flame validation test case, a computational domain of 2 cm containing 10,000 cells (cell size of 2 μm) is considered to evaluate the quenching Peclet number (Peₚ) when the reactants and wall temperatures are equal to 300 K and the pressure is fixed at 1 atm. As previously mentioned, the quenching Peclet number is determined by dividing the quenching distance by the diffusive flame thickness, where the former parameter is the minimum distance between the flame and the wall, and the latter parameter is equal to the ratio of the thermal diffusivity to the unstrained premixed laminar burning velocity. In this test case, the location of the flame is considered to be the iso-contour of temperature occurring at the maximum gradient of the heat release rate in a freely propagating flame. The GRI 3.0 chemical kinetic mechanism [64] containing 53 species and 325 reactions is utilized for this validation test case.

The quenching Peclet number is equal to 2.72 for this test case. This observation is in line with the quenching Peₚ value reported earlier by Owston et al. [15] for the same test case, simulated with the EBiDNSFoam solver [47,48]. They mentioned that the quenching Peₚ value varies from 2.6 to 2.9 using 20 different chemical kinetic mechanisms available in the literature, including the GRI 3.0 chemical kinetic mechanism.

3. Head-on quenching validation test cases

Before discussing the results of the test cases from Table 2, it is of great importance to validate the methodology used in this study for the head-on quenching process. To the best of the authors’ knowledge, there are no experimental results available using ammonia or ammi-

nia/hydrogen flames in the context of head-on quenching that could potentially be utilized for the validation purpose. Thus, our approach in order to tackle this problem is validated using two different single fuel cases. The first validation case is a stoichiometric premixed laminar methane/air flame reported earlier in [12], and the second one is a stoichiometric premixed laminar hydrogen/air flame discussed in [15].

![Schematic representation of the computational domain studied in this work](image-url)
study was equal to 2 μm. As a result, one of the test cases, utilizing the Li chemical kinetic mechanism, is simulated in a domain consisting of 11,200 cells (cell size of 2 μm) to observe whether the quenching distance varies when the cell size value is decreased from 4 to 2 μm. The results indicate a negligible variation of the quenching distance. Therefore, the difference between the quenching distance data of our results and the quenching distance value reported by Owston et al. [15] is not related to the cell size difference. The differences in results are attributed to likely differences in how transport properties are estimated and implemented [68], and/or due to the different chemical kinetic mechanisms utilized herein.

The results presented above, as well as the findings reported in the supplementary material, where the results from one of the test cases studied herein (Case 3 in Table 2) are compared using the reactingDNS and EBDnsFoam solvers (see Fig. B.1), and a comparison is made between reactingDNS and Cantera for a freely propagating premixed ammonia/hydrogen/air flame (Fig. D.1) suggest that the methodology and the reactive flow solver used in the current study are sound. Therefore, it can be utilized for exploring the head-on quenching process of ammonia/air flames enriched with hydrogen with confidence.

4. Results and discussion

In this section, the general overview of the interaction between premixed laminar ammonia/air flames, enriched with hydrogen, and the wall will be examined during the head-on quenching process. This includes a detailed discussion on the quenching distance and the wall heat flux. This section is followed by analyzing the heat release rate profiles and the formation of pollutant emissions (i.e. NO and N₂O species) under different blending ratio, equivalence ratio, wall temperature, and pressure values.

4.1. General overview of the flame–wall interaction

The transient temperature profiles for the reference test case, i.e. Case 3, are shown in Fig. 3(a). In this figure, the normalized time ($r^*$) has been defined as $(t - t_q)/t_{chem}$, where $t$ is the simulation time, $t_q$ is the quenching time, and $t_{chem}$ is the chemical time scale, where the latter time scale is defined as the ratio of the diffusive flame thickness to the unstrained premixed laminar burning velocity. The results show that the flame freely propagates towards the solid wall through initially stagnant reactants (solid lines, $r^* < 0$). Once the flame feels the existence of the solid wall ahead of the flame, the temperature gradient gets larger and the flame thickness becomes thinner. The flame then quenches when the heat loss to the wall is too large (dashed line, $r^* = 0$), and it cannot propagate further towards the solid wall. After quenching, the temperature gradient of the mixture becomes smaller over time (dash-dotted lines, $r^* > 0$). To gain a better understanding of the mentioned process, the temperature in the space–time contour plot for the reference test case is shown in Fig. 3(b). The flame position (solid black line) is defined as the location where the flame temperature is equal to 1500 K. This definition has already been utilized in the literature, see e.g. [13,15,22,69]. The minimum location between the flame position and the solid wall corresponds to the quenching distance (dashed line in Fig. 3(b)). It should be noted that the quantitative values for the quenching distance could vary significantly by using different definitions for the flame location, according to Hasse et al. [13]. However, they emphasized that the time at which the quenching happens is not much dependent on the specific definition.

The quenching distance and the quenching Peclet number values for all the test cases studied in this work are presented in Fig. 4. The variations in each sub-figure are around the reference test case, i.e. all the parameters are held constant except for one parameter that is being changed compared to the reference case. The results presented in Fig. 4(a) show that the quenching distance decreases from approximately 0.5 to 0.2 mm with increasing the blending ratio from 0 to 0.4. The larger the blending ratio, the larger the burning velocity, resulting in a smaller quenching distance. This trend was recently reported by Yu et al. [20] for the same mixture, when the wall temperature is equal to 300 K. The quenching Peclet number increases from 1.72 to 2.03 since the diffusive flame thickness decreases significantly with increasing the blending ratio. The results reported in Fig. 4(b) suggest that both the quenching distance and the quenching Peclet number decrease with increasing the equivalence ratio from 0.8 to 1.2 (quenching distance from 0.33 to 0.2 mm, and quenching Peclet number from 2.9 to 1.75). This observation was previously reported in the literature for premixed laminar hydrogen/air flames, see e.g. [27,52]. Furthermore, Fig. 4(c) shows that increasing the wall temperature from 300 to 750 K results in both the quenching distance and the quenching Peclet number to decrease from 0.34 to 0.09 mm and 3.52 to 1.2, respectively. This observation suggests that the higher the mixture temperature, the higher the initial burning velocity value. Therefore, the flame thickness becomes thinner, and it stagnates closer to the inert wall [22]. Decreasing the quenching distance with increasing the wall temperature was previously observed in the literature for iso-octane flames [13], methane/air flames [16], and hydrogen/air flames [52]. Fig. 4(d) shows that the value of the quenching distance (quenching Peclet number) decreases (increases) from 0.2 to 0.07 mm (2.03 to 2.29) with increasing the mixture pressure from 1 to 5 atm. This observation was previously reported in the literature, see e.g. the experimental measurements performed by Boust et al. [14] and Labuda et al. [19], and the numerical simulations conducted by Westbrook et al. [22] and Yu et al. [20]. The quenching Peclet number values are in a range between approximately 1 and 3.5 for all the test cases in this study. The maximum absolute wall heat flux values for all the test cases studied in the current work are shown in Fig. 5. The results show that the maximum absolute value of the wall heat flux occurs near the quenching time. This trend exists for all the test cases studied in this work. This finding was previously reported by Popp and Baum [17] and Hasse et al. [13].
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Fig. 3. (a) Transient temperature profiles for the reference test case (Case 3). The local Peclet number is defined by dividing the flame distance from the wall by the diffusive flame thickness. (b) Temperature in the space–time contour plot for Case 3. The solid line corresponds to the flame location, and the dashed line shows the quenching distance.

Fig. 4. Quenching distance and the quenching Peclet number with respect to (a) the blending ratio, (b) the equivalence ratio, (c) the wall temperature, and (d) the pressure.

absolute wall heat flux enhances with increasing the blending ratio, the equivalence ratio, the wall temperature, and the pressure. For example, the maximum absolute wall heat flux value is increased from approximately 0.27 to 0.92 MW/m² with increasing the wall temperature from 300 to 750 K. The dependence of wall heat flux on the equivalence ratio and pressure was previously reported by Boust et al. [14], and its dependence on the wall temperature was observed by Hasse et al. [13]. By comparing the quenching distance and the maximum absolute wall heat flux values, it could be concluded that these values are inversely correlated. A similar observation was reported by Zhang et al. [70] for a side-wall quenching setup.

4.2. Heat release rate chemistry

The normalized transient heat release rate profiles are presented in Fig. 7 for the reference test case (Case 3). These heat release rate profiles have been normalized by its maximum value when the flame is far away from the inert wall. The results show that the heat release rate profiles act similar to the heat release rate characteristic of a freely propagating flame, when the flame is outside the vicinity of the wall. Once the flame resides within the influence zone, i.e. a region where the flame is affected by the wall [9], the maximum heat release rate value decreases significantly. The maximum value for the normalized heat release rate decreases to about 0.4 at the instant of quenching, i.e. the time instance when the temperature iso-point reaches closest to the wall. Furthermore, the heat release rate value becomes zero after a certain amount of time after the quenching. A closer look of the variation of the heat release rate profiles in the vicinity of the wall is shown as a sub-figure in Fig. 7. The results show that the heat release rate enhances near the wall at the instant of quenching. This observation was previously reported by several authors in the literature, see e.g. Owston et al. [15].

Following the previous observation, the dimensional heat release rate profiles at the instant of quenching are shown in Fig. 8 for all the test cases. The results clearly suggest a strong dependence of the blending ratio, the equivalence ratio, and the wall temperature on the local heat release rate enhancement near the wall, which is characterized by the small temperature-based progress variable value.
It should be emphasized that increasing the pressure decreases the quantitative value of the local heat release rate near the wall.

To have a clearer comprehension of the above observation, the heat release rate contour plots in the space–time context are shown in Fig. 9(a)–(c), when the equivalence ratio is varied from 0.8 to 1.2. The local heat release rate enhancement near the wall at the instant of quenching is further analyzed by mean of the chemical reaction pathways. This analysis helps to identify the role of important reactions contributing to the heat release rate. The top six reactions contributing to the heat release rate at the position of the maximum heat release rate for the freely propagating flame are shown in Fig. 9(d)–(f). The results show that R144, R3, R27, R35, R190, and R91 contribute significantly to the heat release rate for both the lean and stoichiometric conditions, and R144, R3, R27, R113, R190, and R91 are responsible for most contribution to the heat release rate of the rich mixture. R3, R27, R35, R190, R91, and R113 are chain-propagating reactions, and R144 is a chain-termination reaction. Furthermore, the top six reactions contributing to the heat release rate at the instant of quenching for the first cell near the wall are shown in Fig. 9(g)–(i). In general, the reactions that contribute to the maximum heat release rate, when the flame is far away from the wall, are not mainly active near the cool wall at the time of quenching. The results show that R76 and R22 contribute to the most heat release rate near the wall when the quenching occurs. It is worth noting that R22 is a chain-propagating reaction, and R76 is a chain-termination reaction. Furthermore, R22 is considered as a radical recombination reaction, described by a zero-activation energy. This means that the reaction rate is not significantly affected by the temperature, and its importance is more prominent near the cooler region of the wall, as thoroughly discussed by Owston et al. [15]. The importance of radical recombination reactions on the heat release rate enhancement near the wall was previously reported in the literature, see e.g. Owston et al. [15] and Gruber et al. [21] conducting numerical simulations of premixed hydrogen flames. It should be noted that NO is converted to N$_2$ through R76 which is part of the De-NOx process. This observation will be further discussed in the paper.

Following the observation in Fig. 9(g)–(i), the transient H$_2$O mass fraction profiles are shown in Fig. 10 for the reference test case. The results show that the H$_2$O mass fraction increases considerably near the wall at the instant of quenching. One of the reactions that is responsible for forming this particular species is R22, which is considered a radical recombination reaction. It should be noted that the reaction rate values of the atomic hydrogen are negative, indicating that this species is being consumed near the wall at the time of quenching (not shown for the sake of brevity) through this reaction forming HO$_2$. A similar observation was previously reported in the literature, see e.g. the premixed methane/air flame results explored by Salimath et al. [16] and the premixed hydrogen/air flame results studied by Gruber [52].

4.3. Formation of pollutant emissions

Investigation of the formation of nitric oxide (NO), a component of NOx species, and nitrous oxide (N$_2$O), a component of greenhouse gas, in the vicinity of the solid wall is of great importance due to their harmful effects on the environment. Therefore, studying the formation of these species will be the primary focus of the next two subsections. It should be noted that the magnitude of nitrogen dioxide (NO$_2$), which is a component of NOx species, is very low during the quenching process. Thus, this particular species is not considered in our analysis in the present work.

4.3.1. Nitric oxide formation

Fig. 11 shows the transient NO mass fraction profiles for the reference test case (Case 3). The results show that the maximum value of the NO mass fraction occurs in the high-temperature zone, and it decreases slightly from its maximum value in the post-flame zone before quenching occurs (solid lines, $r^* < 0$). This observation was previously discussed by Karimkashi et al. [6], showing the NO mass fraction profiles of freely propagating ammonia/air and ammonia/hydrogen/air flames in the temperature-based progress variable space. Furthermore, at the time of quenching (dashed line, $r^* = 0$), the NO mass fraction increases moderately in the vicinity of the wall, and it reaches approximately 0.01 after quenching takes place for this particular test case (dash-dotted lines, $r^* > 0$).

Recently, Karimkashi et al. [6] explored the contribution of different reaction pathways in producing/consuming NO for premixed ammonia/air and ammonia/hydrogen/air flames under both laminar and turbulent conditions. Their developed methodology is utilized in this study as well in order to assess the role of each pathway in NO formation before ($r^* < 0$) and at the time of quenching ($r^* = 0$). Similar to the methodology developed by Karimkashi et al. [6], six NO formation pathways are introduced in the current study, namely, HNO, Zeldovich, NO$_2$, NH$_2$, N$_2$, and N$_2$O.

The HNO pathway dictates the formation of NO through HNO intermediate species. The reactions R143 (HNO ⇌ H + NO), R144 (HNO + H ⇌ NO + H$_2$), R145 (HNO + O ⇌ NO + OH), R147 (HNO + OH ⇌ NO + H + O), R148 (HNO + O$_2$ ⇌ NO + HO$_2$), and R149 (HNO + NH$_2$ ⇌ NO + NH$_3$) are part of this pathway. There are more reactions in the Stagni mechanism that could be classified in the HNO pathway, but their contributions in either producing or consuming NO are quite insignificant, at least for these test cases. Therefore, those reactions are excluded from this pathway in the current work. It should be noted that this scenario is valid for other pathways as well. The Zeldovich pathway [71] consists of three reactions. As thoroughly explained by Glarborg et al. [29], the starting step happens when the atomic hydrogen (O) reacts with nitrogen (N$_2$) through R91 (N + NO ⇌ O + N$_2$). The atomic nitrogen (N) also reacts with OH through R89 (N + OH ⇌ NO + H) and O$_2$ through R90 (N + O$_2$ ⇌ NO + O) to form NO. The NO$_2$ pathway is composed of two reactions. The reactions R140 (NO + HO$_2$ ⇌ NO$_2$ + OH) and R181 (H + NO$_2$ ⇌ OH + NO) are considered as the main reactions for this particular pathway.

The NH$_2$ pathway, containing either NH$_2$ or NH radicals as the precursors of NO formation, consists of four reactions. These reactions are R74 (NH + NO ⇌ H$_2$NO + NO), R79 (NH + O ⇌ NO + H), R83 (NH + O$_2$ ⇌ NO + OH), and R116 (N$_2$H$_4$ + NO ⇌ N$_2$O + NH$_2$). According to Karimkashi et al. [6], the N$_2$ pathway consists of four reactions, which lead to the formation of NO through either N$_2$ or NNH species. In this particular pathway, R76 (NH$_2$ + NO ⇌ N$_2$ + H$_2$O), R77 (NH$_2$ + NO ⇌ NH + NO), R86 (NH + NO ⇌ N$_2$ + OH), and R133 (NNH + O ⇌ NH + NO) are considered as the main reactions.
Fig. 6. Maximum absolute wall heat flux values for all the test cases studied in this work.

Fig. 7. Normalized transient heat release rate profiles for Case 3. These profiles have been normalized by the maximum heat release rate value when the flame is far away from the wall. The inset represents a zoom to the near-wall region, and the gray dashed line represents the quenching Peclet number value.

Furthermore, the N\textsubscript{2}O pathway consists of two reactions in this study, namely R85 (NH + NO ⇌ N\textsubscript{2}O + H) and R191 (N\textsubscript{2}O + O ⇌ NO + NO).

The reduction of NO to N\textsubscript{2} is viable through its reaction with NH\textsubscript{i} (i = 0, 1, 2) species [1]. In particular, exploring the De-NOx process, which consumes NO via its reaction with NH and NH\textsubscript{2}, is of great interest through four reactions, namely, R76, R77, R86, and R85. These reactions are classified as part of the N\textsubscript{2} and N\textsubscript{2}O pathways.

The rate of production (rop) of NO through each pathway before the flame interacts with the wall is shown in Fig. 12(a) for the reference test case, Case 3, resulting in the following observations. First, summing the rop of all the pathways (black dashed line) is equal to the total rop of NO (black dash-dotted line). This indicates that the reactions identified in the pathways are capable of capturing the total NO rop.

It should be emphasized that the total NO rop is obtained using all the 41 reactions having NO in the chemical kinetic mechanism utilized in this study. Second, the HNO and N\textsubscript{2}O have the largest roles in the NO rop. The HNO (N\textsubscript{2}O) pathway is responsible for producing (consuming) NO since the rop sign is positive (negative). Furthermore, the NH\textsubscript{2} and N\textsubscript{2} pathways have the lower roles compared to HNO and N\textsubscript{2}O pathways. Third, the Zeldovich and NO\textsubscript{2} pathways have insignificant roles across the flame brush for this particular test condition.

To assess the relative importance of each reaction in the different pathways, Fig. 12(c) shows the NO production rate of each reaction introduced earlier for the pathways before the flame interacts with the wall. The values are obtained at the location where the heat release rate reaches its maximum value, and they have been normalized by the total NO production rate at the same location. The results in Fig. 12(c) show that R144 in the HNO pathway and R85 in the N\textsubscript{2}O pathway have the highest contribution in producing and consuming NO, respectively.

Furthermore, the results show the importance of R91 in consuming NO through the Zeldovich pathway, while its contribution is cancelled by other reactions within the Zeldovich pathway, namely, R89 and R90. The interested reader is referred to Karimkashi et al. [6] for detailed discussion on these pathways for freely propagating laminar ammonia/hydrogen/air flames with different blending ratio values.

Fig. 12(b) shows the rop of NO pathways at the time of quenching for the reference test case. The results confirm that the total NO rop (black dash-dotted line) is equal to the sum of all the pathways (black dashed line). At high temperature, the HNO and N\textsubscript{2}O pathways have the largest roles, and NH\textsubscript{2} and N\textsubscript{2} pathways have the secondary roles similar to the freely propagating flame condition. However, an important observation is that at the lower temperature region, the importance of the HNO pathway, which is the main contributor to NO production in the freely propagating flame, has considerably dropped. In particular, the N\textsubscript{2} pathway, which is the main pathway for NO consumption, has gained significance at the low temperature region closer to the wall, and other pathways present insignificant roles. This indicates that NO is mainly consumed near the wall and this consumption is mainly through the N\textsubscript{2} pathways.

Fig. 12(d) illustrates the rop of NO for each reaction considered in the pathways at the time of quenching for the first cell near the wall. Consistent with the finding shown earlier in Fig. 12(b), the N\textsubscript{2}
pathway has the highest role in the NO consumption in the vicinity of the wall. Within this pathway, R76, which is one of the De-NOx process reactions, has the primary role through which NH$_2$ reacts with NO and produces N$_2$ and H$_2$O. It should be noted that NH$_2$ and NO are abundant in the vicinity of the wall at the time of quenching, which promotes R76. Therefore, the dominance of R76 leads to the conversion of NO to N$_2$ near the wall, which is a desirable process for minimizing NOx emissions, despite its local and, hence, minimal effect in this FWI problem.

To understand the reason behind the high concentration of NO near the wall despite its dominant consumption through chemical reactions, NO transport during the head-on quenching process is analyzed by conducting a species transport budget analysis. This analysis helps to detect the role of the mass convection, molecular diffusion, and reaction source terms in the observed NO concentration. The mass convection is evaluated as $\rho \Delta u Y_i/\partial x$, where $\rho$ is the density, $u$ is the local fluid flow velocity, $Y_i$ is the mass fraction of the desired species $i$, and $x$ is the spatial coordinate. The molecular diffusion is determined by $\partial (\rho D_{mi} \partial Y_i/\partial x + (Y_i/MW) \partial MW/\partial x)/\partial x$, where $D_{mi}$ is the mixture-averaged mass diffusivity of species $i$, and $MW$ is the molecular weight of the mixture. The reaction source term is calculated by multiplying the molecular weight of species $i$ ($MW_i$) to the reaction rate of species $i$ ($\omega_i$).

Fig. 13 shows the mass convection, molecular diffusion, and reaction source terms as well as the mass fraction of NO for the reference test case (Case 3) before the flame interacts with the wall (Fig. 13(a)), at the quenching time (Fig. 13(b)), and after quenching (Fig. 13(c)). The results in Fig. 13(a) show that in the reaction zone region, both of the convection and diffusion terms are negative, and the reaction source term is positive. This observation portrays that the NO is mainly produced within the reaction zone of the flame, and it is diffused and convected out of this zone. A similar observation was thoroughly discussed by Jiang et al. [60] for CO transport of laminar premixed methane flames diluted with hot combustion products. Furthermore, the results in Fig. 13(b) indicate that the diffusion and reaction terms have the dominant roles in NO transport in the vicinity of the wall, and the role of the convection term is negligible. After quenching, the results show that the diffusion and convection terms are positive near the wall, and their sum has a slightly higher value than the negative value of the reaction source term which results in the near-wall NO concentration to increase despite its consumption through R76 near the wall (i.e. the N$_2$ pathway as discussed earlier).

4.3.2. Nitrous oxide formation

As mentioned earlier, exploring the formation of nitrous oxide (N$_2$O) as a potent greenhouse gas is required for ammonia/air flames enriched with hydrogen during the head-on quenching process. Fig. 14 shows the transient N$_2$O mass fraction profiles across the domain for the reference test case (Case 3) before the flame interacts with the wall (solid lines), at the time of quenching (dashed line), and after quenching (dash-dotted lines). The results indicate that the N$_2$O profiles are similar to each other before the flame interacts with the wall, and the authors confirm that these profiles are identical to the N$_2$O profile of an unstrained premixed laminar flame of the same condition (not shown for the sake of brevity). Furthermore, N$_2$O values increase significantly near the wall at the time of quenching ($r^* = 0$), and its values go to zero after quenching, see e.g. the N$_2$O profile at $r^* = 51.56$.

A further analysis shows that among all the reactions having N$_2$O in the chemical kinetic mechanism utilized in this study, two reactions, namely R85 (NH + NO $\leftrightarrow$ N$_2$O + H) and R190 (N$_2$O + H $\leftrightarrow$ N$_2$ + OH), are capable of capturing the total N$_2$O production rate, as shown in Fig. 15(a) for the reference test case before the flame interacts with the wall, and as illustrated in Fig. 15(b) at the instant of quenching. The results show that R85 (R190) is responsible for producing (consuming) N$_2$O across the flame front (Fig. 15(a-b)). The importance of R85 (which is one of the reactions in the De-NOx process) in N$_2$O formation was previously shown by Lindstedt et al. [31] on a set of laminar premixed NH$_3$/H$_2$/O$_2$, NH$_2$/NO/H$_2$/O$_2$, and NH$_3$/O$_2$ flames. Furthermore, the results show that R85 has the dominant role in producing N$_2$O in the vicinity of the wall, while the role of R190 is negligible...
Fig. 9. Heat release rate in the space-time contour (a)–(c), the contribution of important reactions to the maximum heat release rate for the freely propagating flame instant (d)–(f), and the contribution of important reactions to the heat release rate at the instant of quenching in the vicinity of the wall (g)–(i) for Cases 4, 3, and 5. The gray dashed lines in (a)–(c) represent the quenching distance.

Fig. 10. Transient HO\textsubscript{2} mass fraction profiles for the reference test case (Case 3). The inset represents a zoom to the near-wall region, and the gray dashed line represents the quenching Peclet number.

Fig. 11. Transient NO mass fraction profiles for the reference test case (Case 3). The inset represents a zoom to the near-wall region, and the gray dashed line represents the quenching Peclet number.
Fig. 12. Rate of production (rop) of NO for Case 3 (a) before the flame interacts with the wall, and (b) at the time of quenching. NO production rate of the reactions identified in the pathways for Case 3 (c) before the flame interacts with the wall, and (d) at the time of quenching. The data for (c) are captured at the location where the heat release rate reaches its maximum value, and the data for (d) are obtained at the first cell near the wall. The values for the last two sub-figures have been normalized by the total NO rop.

Fig. 13. NO transport budget analysis and mass fraction with respect to the local Peclet number for Case 3, (a) before the flame interacts with the wall, (b) at the time of quenching, and (c) after quenching. The gray dashed lines in (a)–(c) show the quenching Peclet number. (see the zoomed sub-figure in Fig. 15(b)). Fig. 15(c)–(f) shows the total $N_2O$ production rate of all the test cases in the temperature-based progress variable space. The results suggest that $N_2O$ increases locally at the low progress variable value, which is translated into the near-wall location in the space-coordinate system, with increasing the blending ratio (Fig. 15(c)), the equivalence ratio (Fig. 15(d)), and the wall temperature (Fig. 15(e)). However, increasing the pressure up to 5 atm does not seem to have a noticeable effect on the aforementioned observation (Fig. 15(f)).

Fig. 16 shows the $N_2O$ transport budget terms and its mass fraction during the head-on quenching process. Before the flame interacts with the wall, the $N_2O$ produced across the flame is diffused and convected out from the production zone as shown in Fig. 16(a). At the time of quenching, Fig. 16(b), the diffusion term has the dominant role in enhancing the $N_2O$ transport in the vicinity of the wall, and the role of the reaction source term in increasing the near-wall $N_2O$ transport is also considerable within the quenching region. However, the role of mass convection is negligible. After quenching, Fig. 16(c), all the transport budget terms go to zero, and they do not contribute to the $N_2O$ transport anymore.

It should be borne in mind that the current study is performed for the head-on quenching process, which is potentially different than the side-wall quenching process for ammonia flames. Therefore, examining the side-wall quenching process of ammonia-blended flames is of great interest, which will be the foundation of future explorations.

5. Concluding remarks

The transient normal interaction between premixed laminar ammonia/air flames enriched with hydrogen and the wall (head-on quenching) was explored using numerical simulations with detailed chemistry using the mechanism developed by Stagni et al. [35] and the mixture-averaged transport model. In this study, nine different head-on quenching test cases were studied in detail. The blending ratio, indicating the hydrogen concentration in the ammonia/hydrogen mixture, was systematically varied from 0.0 to 0.4. Furthermore, the equivalence...
Fig. 14. Transient N\textsubscript{2}O mass fraction profiles for the reference test case (Case 3). The inset represents a zoom to the near-wall region, and the gray dashed line illustrates the quenching Peclet number.

Fig. 15. Rate of production of N\textsubscript{2}O through R85, R190, R85+R190, and all the reactions containing this species in the chemical kinetic mechanism utilized in this work, (a) before the flame interacts with the wall, and (b) at the time of quenching. Total N\textsubscript{2}O production rate with respect to the temperature-based progress variable when investigating the effect of (c) the blending ratio, (d) the equivalence ratio, (e) the wall temperature, and (f) the pressure at the instant of quenching.
ratio, the wall temperature, and the pressure were changed between 0.8 and 1.2, 300 and 750 K, and 1 and 5 atm, respectively. The main findings of the current study are outlined as follows:

(1) The results showed that the quenching distance decreased with increasing the blending ratio, the equivalence ratio, the wall temperature, and the pressure. For all the test cases studied in this work, the quenching Peclet number values are in a range between 1 and 3.5. Furthermore, the results indicate that the maximum absolute wall heat flux values increased with increasing the blending ratio, the equivalence ratio, the wall temperature, and the pressure.

(2) The variation of heat release rate during the head-on quenching process was explored, and the important reactions contributing to the heat release rate during this process were detected. In addition, the local heat release rate enhancement and the major role of radical recombination reactions for this enhancement were discussed at the time of quenching in the vicinity of the wall. The results showed that this local heat release rate enhancement is amplified with increasing the blending ratio, the equivalence ratio, and the wall temperature.

(3) The formation of NO and N₂O was discussed during the head-on quenching process. Furthermore, the reactions contributing to the production/consumption of these species were analyzed before the flame interacts with the wall and at the time of quenching. The results indicated that NO converts to N₂ and also N₂O to some extent in the vicinity of the wall at the time of quenching. The results revealed that among different pathways contributing to the production/consumption of NO, the N₂ pathway was detected to be the leading pathway in consumption of NO near the wall at the time of quenching, and R76 (NH₂ + NO ⇌ N₂ + H₂O) was determined to be the dominant reaction within this pathway. Further, the primary role of R85 (NH + NO ⇌ N₂O + H) in forming N₂O in the vicinity of the wall was shown at the time of quenching.

(4) The transport budget analysis was performed for both NO and N₂O species to explore the role of mass convection, molecular diffusion, and reaction source terms during the head-on quenching process. The results showed that the NO was produced within the reaction zone of the flame, and it was diffused and convected out of this zone before the flame interacts with the wall. In the vicinity of the wall, the chemistry was responsible for consuming NO and converting it to N₂, while the NO was diffused in this region at the time of quenching. Furthermore, the N₂O which was produced across the flame was diffused and convected out from the production zone before the flame interacts with the wall. In the close proximity of the wall and at the instant of quenching, the diffusion had the dominant role in enhancing the N₂O transport, and the role of chemistry was significant within the quenching region.

CRediT authorship contribution statement

Parsa Tamadonfar: Formal analysis, Investigation, Methodology, Software, Conceptualization, Writing – original draft, Writing – review & editing. Shervin Karimkashi: Investigation, Writing – review & editing. Thorsten Zirwes: Investigation, Software, Writing – review & editing. Ville Vuorinen: Supervision, Writing – review & editing. Ossi Kaario: Funding acquisition, Methodology, Conceptualization, Supervision, Writing – review & editing.

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.

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Appendix A. Supplementary data

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