Effects of n-decane substitution on structure and extinction limits of formic acid diffusion flames

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Formic acid (FA) is a low-carbon fuel that can be produced from renewable hydrogen (H\textsubscript{2}) and carbon dioxide (CO\textsubscript{2}). However, transitioning completely to low carbon fuels might be lengthy and challenging, so it makes sense to gradually introduce low carbon fuels into the energy sector in conjunction with existing fuels. One practical approach could be blending FA with existing fossil fuels, such as kerosene in aviation. This study investigates the behavior of flames comprising FA and its blends with n-decane. The extinction limits of pure FA and FA/n-decane mixtures were measured in a counterflow non-premixed laminar flame setup at various blending ratios. Additionally, the flame structure was studied by measuring temperature and species distribution using probe-based sampling. The results indicate that replacing FA with n-decane in the FA-N2 flame greatly enhances the flame's reactivity. Blending the fuels also led to a decrease in CO\textsubscript{2} production in the flame, while increasing the flame temperature and the concentration of H\textsubscript{2} and CO species. Experimental results were modeled using an updated FA and n-decane model. The kinetic model agrees with the experimental trends, but slightly overpredicts H\textsubscript{2}, CH\textsubscript{4} species, and flame temperature. The kinetic model was also used to investigate the kinetic coupling between FA and n-decane in non-premixed laminar flames. Kinetic analyses indicate that HOCO and OCHO intermediates play a crucial role in pure FA flames by reacting with active radicals like H and OH to produce CO\textsubscript{2} and CO, while in n-decane blended flames, fuel decomposition proceeds through two other pathways leading to H\textsubscript{2} and H\textsubscript{2}O\textsubscript{2}.

Key Words: Formic Acid; Flame Extinction; non-premixed flames; Counterflow flames
1.0 Introduction

The rise in global energy consumption has led to a significant increase in greenhouse gases and pollutants such as unburned hydrocarbons, carbon monoxide, and nitrous oxides. Emissions resulting from burning fossil fuels in the transportation and power industries constitute 50% of the overall greenhouse gas emissions in the United States [1]. To meet the climate ambitions stated by many countries, there is a need to shift to lower carbon and sustainable fuels.

As the world races to adopting clean energy source, hydrogen is often viewed as a promising energy carrier and fuel. Hydrogen burns without carbon-related emissions. However, hydrogen is a gas at room temperature and highly flammable, which render it difficult to transport and store. One solution is to use a hydrogen carrier such as ammonia (NH$_3$) or formic acid (FA) to store and transport hydrogen. Compared to pressurized hydrogen, formic acid (FA) is liquid at room temperature and can store almost twice as much energy at equal volume [2, 3]. This allows for a more compact design of storage tanks in vehicles. Formic acid can be produced from renewable H$_2$ and captured CO$_2$, biomass decomposition, or as an industrial by-product via photoelectric catalytic reduction of CO$_2$ [4, 5]. Formic acid decomposes at mild temperature conditions to release H$_2$, which is an important attribute for on-demand release and utilization in vehicles that are using hydrogen fuel cells [2].

The development of models that could be used to understand the combustion behavior of any candidate fuel in realistic energy systems, relies on fundamental experimental data for validation. These data include flame speed, ignition delay time, flame extinction and speciation. However, as mentioned recently by Sarathy et al. [4], most previous studies on FA focus on understanding its decomposition behavior in shock tube and flow reactors, and only a few reported its flame behavior. Marshall et al. [6] developed a detailed kinetic model for FA oxidation. They tested their model using old laminar burning velocity (LBV) data by Wilde et al. [7] in a Bunsen burner configuration. Their model over-predicted the experimental
measurement, especially under rich conditions. Sarathy et al. [4] developed a FA kinetics model by merging the FA sub mechanism with Aramco 2.0 base chemistry and measured the LBV of mixtures containing HOOCOOH, H₂, and CO₂ in spherical flames. They compared their measurements using both Marshall et al. [6] mechanism and their own mechanism. Their developed mechanism better reproduces the experimental trend, especially under lean and stoichiometric conditions. Osipova et al. [8] used the molecular beam mass spectrometer to measure the laminar premixed flame structure of HCOOH/H₂/O₂/Ar in a flat flame burner. Both models, developed by [6, 9], captured the mole fractions of the reactants, but over-predicted the concentration of H₂, H₂O₂ and HO₂ species.

Lavadera et al. [10] measured the LBV of FA+CH₄+Air flames using the heat flux method and noted disparities in their measured flame speed with the data reported by Yin et. al. [11], especially under rich conditions. They updated the Glarborg et al. [6] mechanism by modifying the rate constant for HOOCO(+M)=H+CO₂(+M), which significantly improved the performance of the model even at rich conditions. In another study, Yin et al. [12] used a high-level quantum calculation to obtain the rate coefficients of missing reactions in Glarborg et al. [6] kinetic mechanism. They developed a detailed chemical kinetic mechanism that includes low temperature oxidation and pyrolysis reactions of FA. Their model reproduced speciation data from FA pyrolysis and oxidation in JSR and flame speed data by [4, 11] under rich and lean conditions.

All previous studies focused on flame speed data and were performed in homogeneous systems where the effects of transport are negligible. In practical combustion systems such as turbines and compression ignition engines, combustion takes place in the presence of concentration and temperature gradients, such that reactants and intermediate products diffusion can affect the
reaction kinetics, and therefore, can contribute to flame propagation, emission and stability [13-17].

The low LBV of FA is a drawback as a potential fuel for practical applications. As a result, many studies have explored blending FA fuel with reactivity promoters such as CH₄, H₂, and H₂/CO₂. A similar procedure is used for low reactivity hydrogen-carrying fuels such as ammonia [18-21]. The aim of this study is to investigate the potential of formic acid as a fuel source by analyzing its behavior in non-premixed diffusion flames. The counterflow configuration is used to understand the flame stability of FA and its blends with n-decane (nC₁₀H₂₂), a relevant surrogate fuel for kerosene in combustion research [22, 23]. The extinction limits of both pure FA flame and flames of FA/n-decane blends under various conditions will be measured. The flame structure will also be analyzed by measuring temperature and species distribution using gas chromatography. Additionally, the study tests the predictive capability of a recently developed chemical kinetics model for these fuel blends [12] in non-homogeneous environments, such as those found in turbines.

2 Description of the Experimental and Numerical Procedure

2.1 Experimental Procedure

Figure 1 shows a schematic illustration of the counterflow configuration used in this study. The burner consists of two opposing ducts, each having an internal diameter of 20 mm. The upper burner carries an oxidizer stream, while the lower burner contains the fuel stream. These jets flow into the mixing layer between the two ducts. The fuel stream in this case comprises the fuel (pure FA, pure n-decane or FA + n-decane mixture) and nitrogen. The liquid fuel is injected using a high precision syringe pump. The liquid fuel is first vaporized and then introduced into the counterflow system. A thermocouple is used to monitor the temperature of the fuel stream inside the vaporizer and at the exit of the fuel outlet. The flow rates of air and nitrogen are...
adjusted by computer-regulated mass flow controllers. The two ducts are separated by a distance \( L \). The fuel mass fraction, temperature, density of the fuel stream, and the component of the fuel flow velocity normal to the stagnation plane at the exit of the fuel outlet were \( Y_{f,1}, T_1, \rho_1, \) and \( V_1 \), respectively. The oxygen mass fraction, oxidizer temperature, density, and the oxidizer flow velocity normal to the stagnation plane at the exit of the oxidizer outlet were \( Y_{O2,2}, T_2, \rho_2, \) and \( V_2 \), accordingly. All experiments were conducted assuming plug flow conditions and keeping the momenta of the counterflowing streams equal (\( \rho V_i = 1,2 \)). The strain rate, \( a_2 \), Eq. (1), is defined as the gradient of the normal component of the flow velocity [24].

\[
a_2 = \frac{2|V_2|}{L} (1 + \frac{|V_1|\sqrt{\rho_1}}{|V_2|\sqrt{\rho_2}})
\] (1)

Extinction experiments were carried out at \( T_2 = 298 \) K, and \( T_1 \) kept close to the boiling point of the fuel mixture. To measure the extinction limits, the flame is stabilized at a given fuel and oxidizer mass fraction \( Y_{f,1}, \) and \( Y_{O2,2} \). Subsequently, the velocities \( V_1 \) and \( V_2 \) were gradually increased by increasing the flow rates while maintaining a balanced momentum between the two counterflowing streams until the flame was extinguished. The corresponding strain rate at extinction, \( a_{2,E} \), is then calculated using Eq. (1) above. The strain rate at stable flaming condition is lower than the extinction strain rate. The process is repeated to verify each data point. The accuracies of the strain rate was estimated at 7% of the recorded values. The experimental repeatability of the reported strain rate at extinction was 3% of the recorded value. The flame temperatures were measured using an Omega (Pt/10% Rh-Pt) thermocouple with a wire diameter of 0.075 mm. The measured temperatures are corrected according to [25, 26] by considering the heat transfer due to radiation and convection between the thermocouple bead and the surrounding.

The gas products were quantified using a gas chromatograph (GC, Thermo Scientific TRACE 1610). The GC was fitted with two pre-columns (Porapak N), two analytical columns (5Å MoleSieve), one mixed pre-column (TG-WAXMS+TR-1), one HP AL/S column, and two TCDs and one FID. Ultra-high purity He and N\(_2\) were used as carrier gases. The gas product
was injected directly into the sampling loop of the GC by a vacuum-assisted gas sampling system. The TCD and FID detectors showed good linearity over a wide concentration range toward \( \text{H}_2 \), \( \text{O}_2 \), \( \text{CO} \), \( \text{CO}_2 \), \( \text{CH}_4 \), \( \text{C}_2\text{H}_2 \), \( \text{C}_2\text{H}_4 \), and \( \text{C}_2\text{H}_6 \). The error for \( \text{H}_2 \) speciation is less than 5%. Similarly, the errors for \( \text{CO} \), \( \text{CO}_2 \), and hydrocarbons are less than 4.0%.

### 2.2 Numerical Procedure

The Yin et al. [12] mechanism for FA, was used for the simulation. The mechanism was extended to include the recently developed reaction mechanisms for n-decane. Brunialti et al. [27] developed a methodology for automatic generation of predictive lumped and detailed mechanisms for normal and branched alkanes including n-decane. A comprehensive detailed reaction mechanism for combustion of alkanes was generated by employing an updated version of MAMOX++ software, where recent progress in the low temperature reaction classes and rate rules are incorporated. The developed kinetic mechanism agreed well with experimental data in the literature, including the speciation data measured in the JSR and global ignition delay times [28-30].

Extinction simulations were carried out using the 1-D extinction solver on CHEMKIN-PRO. The solver uses an arc length continuation method to generate the S-curve [16, 31]. The procedure involves establishing a stable flame using the OPPDIF code at conditions close to extinction, and then the solution is restarted in the extinction solver. A 2-point extinction method with 1000 steps was used. Convergence factors \( \text{GRAD} \) and \( \text{CURV} = 0.1 \) were used to control the maximum gradients and curvatures allowed between grid points. The multicomponent mixture formulation was used to determine species diffusive coefficients and fluxes.
3 Results and Discussion

3.1 Extinction measurement

For validation purposes, the extinction strain rates of n-decane-N\textsubscript{2} were measured and compared to previous experimental data by Humer et al. [32]. The results are shown in Fig. 2. Overall, the present experimental results show a good agreement with the previous data. As Formic acid exhibits low reactivity, it cannot sustain a flame in air. Consequently, an oxidizer enriched with oxygen (X\textsubscript{O2}=0.5) is employed to determine its extinction limit (see Fig. 2). As illustrated in Fig. 2, the extinction limit of both flames increases as the fuel mass fraction is increased. FA-N\textsubscript{2} flame is more prone to extinction as compared to n-decane-N\textsubscript{2}. Extinction limit measures flames' resistance to local extinction; therefore, flames with higher extinction limits are more resistant and correspondingly more stable. In other words, the area under the lines in Fig. 2 represents a stabilized and burning flame region. Above the lines, the flame cannot withstand the leakages of heat and radicals, and therefore the flame is extinguished. This trend in reactivity of FA results also agree with results reported by Sarathy et al. [4] where they reported a very
low LBV for formic acid. Worth noting is that n-decane has more active sites for H\textsubscript{2} abstraction, and when it reacts in flames it populates active radicals which sustain the flame.

Figure 2. The extinction strain rate $a_{2,E}$ as a function of the fuel mass fraction for FA-N\textsubscript{2} and n-decane-N\textsubscript{2} fuels. Purple and Red stars are present measurements, while red circles are measurements from Humer et al., 2007 [32]. Lines are numerical simulations.

Figure 3 shows the dependence of the extinction strain rate on the fuel mass fraction for nitrogen-diluted n-decane/air and n-decane blended FA/air flames. The blending ratio is defined as the liquid volume ratio between n-decane and FA, and this is systematically varied from 10% n-decane (i.e. 90% FA) to 100% n-decane. The results show an increase in the reactivity of FA-N\textsubscript{2} flame as more FA is substituted by n-decane in the mixture. This shows the ability of n-decane to improve the flammability limit of FA in opposed flow diffusive systems. Also as illustrated in Fig. 3, the model agreed with the observed experimental trend for both fuel mixtures. The flame structure and kinetic analysis below rationalize why the extinction strain rate of FA is significantly affected by n-decane substitution.
Figure 3. Mass fraction of fuel as a function of strain rate at extinction, $a_{2,E}$ in the counterflow diffusion flame. Symbols represent experimental measurement, dash-dot lines represent modeling predictions.

3.2 Measured and simulated flame structure

Figure 4 illustrates the temperature measurements along with the measured concentration profiles of CO, CO$_2$, and H$_2$ for two types of flames: FA-N$_2$ and a 30% n-decane substituted flame. These measurements were conducted at strain rate = 41 s$^{-1}$ with an oxidizer containing 50% O$_2$. The H$_2$ concentration and temperature of the nitrogen-diluted FA flame showed a significant increase upon the substitution of 30% n-decane into the fuel stream. Additionally, the n-decane substituted flame exhibited a higher concentration of CO and H$_2$ compared to the FA-N$_2$ flame. The impact of CO on the observed higher reactivity of the substituted flame is analyzed in detail in the following section. It is worth noting that the maximum concentration of CO$_2$ in the nitrogen-diluted FA flame was found to be approximately 21000ppm, whereas it reduced to 18000ppm with n-decane substitution.
Figure 4. Measured temperature and species concentration of laminar non-premixed counterflow flames with the fuel blends. Blue lines and symbols represent the profiles for the n-decane substituted flame, and black lines and symbols represent the profiles for the FA-N2 flame. The vertical error bars represent the errors related to the concentration results; the horizontal error bars represent the errors related to the probe sampling position, which are ± 0.075 mm for each experimental data.

Figure 5a presents both simulated and measured temperature and species concentration profiles for FA-N2 flame. The model quantitatively reproduces CO$_2$ concentration profiles, but it over-predicts the measured temperature and species of H$_2$ and CO in the FA-N2 flame. Similarly, Fig. 5b illustrates the measured and simulated flame structure of n-decane substituted flame. The model reproduces CO$_2$, CO, C$_2$H$_2$, C$_2$H$_4$ species but slightly overpredicted flame temperature and CH$_4$ concentration. Moreover, a better agreement is observed for H$_2$ in comparison to the FA-N2 flame in Fig. 5a.
Figure 5a. Measured and simulated flame temperature and species concentration of FA-N2 flame. Lines are numerical simulation while symbols plus lines are experimental measurements. The vertical error bars represent the errors related to the concentration results; the horizontal error bars represent the errors related to the probe sampling position, which are ± 0.075 mm for each experimental data.
Figure 5b. Measured and simulated flame temperature and species concentration of n-decane substituted flame. Lines are numerical simulation while symbols plus lines are experimental measurements. The vertical error bars represent the errors related to the concentration results; the horizontal error bars represent the errors related to the probe sampling position, which are ± 0.075 mm for each experimental data.

3.2.1 Effects of n-decane substitution on fuel consumption

Reaction path flux analyses were performed at 65% fuel consumption to compare fuel consumption pathways between the FA-N\(_2\) and the n-decane substituted FA flames as illustrated in Fig. 6. The 30% n-decane substituted FA flame is used. These analyses were conducted under the same conditions depicted in Fig. 5. For the FA-N\(_2\) flame, approximately 76% of the fuel decomposition proceed via HOCO intermediate route, where FA undergoes H abstraction reaction by OH and H to produce H\(_2\)O and H\(_2\) as the secondary products. Around 24% of FA consumes hydroxyl radical (OH) to produce OCHO and H\(_2\)O. About 94% of HOCO intermediates in the FA-N\(_2\) flame dissociated into OH and CO, while the remaining react with
hydrogen radicals (H) to produce H$_2$O and CO. Almost 100% of OCHO intermediate dissociates into CO$_2$ and H radicals.

In the 30% n-decane substituted FA flame, two additional pathways were observed: about 4.3% of the fuel dissociated directly into H$_2$ and CO$_2$, and 5.6% of the fuel reacted with hydroperoxy radicals to produce HO$\cdot$CO and hydrogen peroxide. The remaining fuel proceeded through the pathways of HO$\cdot$CO and OCHO intermediates to generate CO, CO$_2$, and other secondary radicals.

The primary difference between these flames is related to the consumption of FA and of course, the presence of n-Decane fragments. In FA-N$_2$ flames, fuel decomposition primarily involves HO$\cdot$CO and OCHO intermediates that consume H and OH active radicals to produce CO and CO$_2$. In contrast, two other pathways leading to H$_2$ and H$_2$O$_2$ production were observed in the 30% n-decane substituted FA flame. The remaining fuel in this case proceeded through the chain propagation route to produce HO$\cdot$CO, which further reacted to yield CO and CO$_2$.

Increasing the CO, OH, and H concentration increases the rate of heat release in the flame through the CO+OH=CO$_2$+H and H+O$_2$=OH+O reactions, as demonstrated in the sensitivity analyses shown in the later section. Additionally, in the FA-N$_2$ flame, 6.8% of CO was consumed via the HCO formation route (CO+H+M$\rightleftharpoons$HCO+M), with most of the HCO reacting with O$_2$ to produce HO$_2$ and CO again. Moreover, while 100% of HO$\cdot$CO produced CO and OH in the 30% substituted n-decane flame, around 3.7% and 2.5% of HO$\cdot$CO reacted with H radicals to respectively produce CO, CO$_2$ and H$_2$O in the FA-N$_2$ flame. Overall, the radicals-scavenging reactions observed in FA-N$_2$ flames, along with the pathways leading to the production of H$_2$O$_2$ and H$_2$ observed in n-decane blended flames, could provide an explanation for the lower reactivity in FA-N$_2$ flames and the increase in reactivity resulting from n-decane substitution.
Figure 6. Reaction flux analyses showing major pathways for fuel and intermediates consumption. Red are percentages for FA flame, gray represents percentages for the 30% n-decane substituted FA flame.

To understand which reactions affect the extinction limits of the FA-N₂ and 30% n-decane substituted flames, brute force sensitivity analyses were conducted and are presented in Fig. 7. The analyses used percentage sensitivity [33, 34], which is defined as:

\[
\% S = \left( \frac{a_{EI} - a_{Enorm}}{a_{Enorm}} \right) \times 100
\]  \hspace{1cm} (2)

where \( a_{EI} \) is the extinction strain rate when the rate constant is doubled (\( k = 2k \)) and \( a_{Enorm} \) is the extinction strain rate for an unchanged rate in the mechanism.

Prior to the brute force sensitivity analyses, a temperature sensitivity analysis was performed under the same conditions to identify the most sensitive reactions [35]. Increasing the rate of reactions with positive sensitivity enhances reactivity, resulting in higher extinction limits, while decreasing their rates decreases reactivity and vice versa. Both flames are positively impacted by branching reactions that produce O, OH, and H radicals. They are also sensitive to heat-producing reactions such as CO+OH ⇋ CO₂+H. Although not shown in Fig. 7, this reaction...
accounts for most of the heat released in the FA-N\textsubscript{2} flame. The FA-N\textsubscript{2} flame's reactivity is negatively impacted by FA fuel fragments, especially HOCHO+OH $\rightleftharpoons$ HOCO+H\textsubscript{2}O and HOCO+H $\rightleftharpoons$ CO+H\textsubscript{2}O. In this case, OH is consumed to produce HOCO and H\textsubscript{2}O, which scavenges H radical to form CO and H\textsubscript{2}O. As previously discussed in the reaction flux analyses, subsequent CO reactions in the FA-N\textsubscript{2} flame result in the formation of HCO, which reacts with H radicals to produce HO\textsubscript{2} and CO. In contrast, HOCO producing reactions are positively sensitive in the n-decane substituted flame, where nearly 100\% of HOCO proceeds through the CO and OH formation route. As shown in Fig. 7, the n-decane substituted flames are negatively affected by beta-scission products of n-decane fragments, which produce intermediates that undergo subsequent reactions to produce highly branched and resonantly stable products.

![Figure 7. Sensitivity analysis of FA-N\textsubscript{2}, and n-decane substituted flames to extinction](image)

### 3.2.1 Effects of n-decane substitution on FA flame structure

The simulated species profiles in Fig. 5 are combined and shown as illustrated in Fig. 8, in order to trace the fuel consumption, radicals formation and production of CO/CO\textsubscript{2} species. The maximum flame temperature for FA-N\textsubscript{2} flame is ~1600K, however with n-decane substitution, the flame temperature increase by more than 400K. The lower flame temperature in FA-N\textsubscript{2} flame is related to the lower calorific value of the flame leading to lower active radicals, which...
decreases the overall reactivity of the flame. It is worthy to note that H, OH, and O radicals are higher in the n-decane substituted FA flame, and can diffuse across the stagnation plane to sustain the flame, by initiating more fuel abstraction. This improves the flames’ stability and increases its resistance to extinction. It can be seen in Fig. 8, that the fuel and the oxidizer are consumed earlier in the n-decane substituted flame, which is an indication of fast oxidation as a result of the enhanced activity of the radicals produced by the flame.

**Figure 8.** Effects of n-decane substitution on the structure of the FA flame. Dashed line represents the FA-N$_2$ flame; while straight lines are 30%, n-decane substituted flame. Simulation are carried out at strain rate ($41 \text{ s}^{-1}$), $Y_F = 0.5$ and $X_{O_2}$ in oxidizer is 0.5.

### 4.0 Conclusions

The present study investigated the flame structure of formic acid (FA) and n-decane blends in a counterflow laminar non-premixed flame configuration. Both experimental and simulations were conducted in this study. The results indicate that replacing FA with n-decane in the FA-N$_2$ flame greatly enhances the flame's reactivity of FA-based flames and reduces CO$_2$ production while increasing the concentrations of H$_2$ and CO species in the flame. The experimental results were simulated using Yin et al. chemical kinetics mechanism [12], which was extended to include Brunialti and Zhang et al.’s [27] n-decane sub-chemistry. The model was in good agreement with the measured extinction limits and flame structure, and helped to
elucidate the kinetic coupling between FA and n-decane in non-premixed laminar flames. Results from kinetic analyses revealed that HOCO and OCHO are important intermediates for the FA-N₂ flames, while n-decane blended flames decompose through two additional pathways leading to H₂ and H₂O₂ formation. Sensitivity analyses showed that both types of flames are sensitive to heat-producing and branching reactions, as well as H abstraction reactions of FA by OH radical. The FA-N₂ flame is negatively sensitive to HOCO radicals producing reactions, while n-decane substituted flames show positive sensitivity as nearly 100% of HOCO reactions, the flame proceeds through the CO and OH formation route. The 30% n-decane substituted flame is also sensitive to reactions involving n-decane fuel fragments. Finally, the n-decane substituted FA flame exhibited the highest extinction limit due to its higher flame temperature and concentration of active radicals. These findings provide valuable insights into the viability of FA and its blends, with higher hydrocarbons as potential alternative fuel sources for practical applications.

**CRediT authorship contribution statement**


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