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A Kinetic Modeling Study for the Effect of NO_x on Oxymethylene ethers (OME_n, n = 0 and 1) oxidation

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Abstract

We present a detailed kinetic model for the oxidation of dimethyl ether (OME₀) and dimethoxymethane (OME₁) in presence of NO_x. We further explored the effect of NO_x chemistry on the oxidation kinetics of the two OMEs. Our kinetic model is validated against the recent flow reactor data from Zhang et al. (Combust. Flame. 224 (2021) 94–107). The results indicated that NO doping severely alters the oxidation kinetics of both fuels. The onset temperature for total fuel consumption is significantly shifted to lower temperatures for both fuels, which is in line with the experimental observation. We found that the addition of NO significantly inhibited the NTC behaviour of dimethyl ether. This inhibiting effect appears to stem from the competition between CH₃OCH₂O₂ radical consumption by NO directly and the isomerization/dissociation reactions of CH₃OCH₂O₂. Unlike dimethyl ether, dimethoxymethane does not exhibit a strong NTC behavior, and NO addition completely inhibited its weak NTC behavior.

Introduction

For future sustainability, carbon-neutral fuels can be key platform chemicals to achieve zero net CO₂ emission. They can be produced from renewables feedstocks and synthetic gas in a sustainable carbon cycle (see ref.1 (Fuel 291 (2021) 120217) and references cited therein). Among carbon-neutral fuels, the oxymethylene ethers (CH₃O(CH₂O)_nCH₃, OME_n) are particularly interesting fuel candidates for several reasons. They possess a high cetane number, high oxygen content, and no C–C bonds which allows for soot-free and low-NO_x combustion. The number of oxymethylene groups (n) influences the properties of the fuel. If n is increased, the cetane number rises, and diesel-like boiling temperatures are reached [1,2]. Additionally, OMEs are non-toxic making them good candidates for blending with diesel fuel. Such blends have shown a significant reduction of soot emissions [3,4]. Soot emissions were reduced when oxygenated hydrocarbons were blended with regular diesel fuel [5]. The amount of fuel-born oxygen has a direct correlation with the propensity of soot reduction. It was found that each fuel-born oxygen of the oxygenated species added to the fuel has approximately the same effectiveness in reducing soot emissions, but it does not depend on the chemical nature of the oxygen-containing species (see Ren et al. [4] and Natarajan et al. [6])

The oxidation chemistry of dimethyl ether (DME, OME₀) has been extensively studied [7–9]. In CI engines exhaust products are often recirculated to the combustion chamber. The use of oxygenated fuels in CI engines in neat or as additives requires the fundamental understanding of fuels and NO_x interaction. The complex fuel-specific chemical interactions between fuel and NO are still not well understood. Most earlier studies focused

to explore the interactions between hydrocarbons and NO, while studies on emerging renewable alternative fuels are still limited. Unlike hydrocarbon-fuel/NO_x system, studies related to the oxygenated-fuel/NO_x system are scarce. To our knowledge, only a few studies are rendering to DME/NO_x system to date [10–13]. As discussed earlier, OMEs produce less NO_x due to less favorable conditions for thermal NO formation. For this reason, the NO_x effect on the oxidation kinetics of OMEs did not receive much attention. However, NO_x is also one of the by-products along with other exhaust products during fuel combustion.

In a recent work [14], we carried out a detailed kinetic modeling study by investigating NO_x interaction during the oxidation of methanol and ethanol. Here, we extend our campaign by investigating the sensitizing effect of NO_x on the oxidation kinetics of dimethyl ether (OME₀) and dimethoxy methane (OME₁). Recently, Zhang *et al.* [15] studied NO interaction with dimethyl ether (DME, OME₀) and dimethoxymethane (DMM, OME₁) in a flow reactor. They simulated their experimental results by using four different kinetic mechanisms from the literature including the one from our recent study [16]. They reported that none of the available mechanisms adequately captured the experimental data. This observation warranted additional work aiming to improve the predictive capabilities of the kinetic model. Our aim is to improve our recently published mechanism [17] and provide a better understanding of the combustion behavior of DME (OME₀) and DMM (OME₁) in presence of NO_x. Such study will serve as a baseline for the understanding of NO_x interaction kinetics with larger OME_n (n>1).

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Chemical kinetic modeling

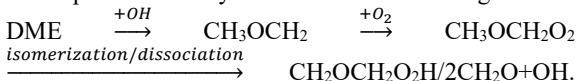
The mechanism proposed here builds upon our recent work on the oxidation kinetics of DME and DMM, and their interactions with NO_x chemistry [17]. We validated our kinetic model [17] against various experimental targets of the chemical systems comprising C₁-C₂ fuels. Our kinetic model satisfactorily captured the oxidation kinetics of C₁ - C₂ hydrocarbons/oxygenates - NO_x chemistry interaction as well as NO formation in C₁ - C₂ premixed flames. However, we could not test our model against DMM/NO system due to the unavailability of the experimental data at that time. Therefore, we added new reaction pathways to improve the predictive capabilities of our kinetic model describing the low-temperature oxidation chemistry of DME and DMM and their interactions with NO_x chemistry. We employed LOGEresearch v1.10.0 [18] software package for all kinetic simulations.

Results and Discussion

As stated earlier, our study particularly emphasizes on DME/NO_x and DMM/NO_x system. The performance of our kinetic model is compared with the recent experimental data from Zhang et al. [15]. Unless stated otherwise, the lines in the figures below represent the simulation results of this work; whereas the symbols represent the experimental data from Zhang et al. [15].

NO_x chemical effect on DME Oxidation

Figure 1 compares the model predictions with the experimental data. The experimental data were taken from Zhang et al. [15] who investigated the oxidation kinetics of DME and DMM with/ without NO (0, 1000, 2000 ppm) in a plug-flow reactor over the temperature range of 400-1000 K, the pressure of 1 atm and $\phi = 0.8$. As seen in Figure 1a, the onset of DME oxidation without NO occurs at ~510 K. Interestingly, the presence of NO shifts the onset of DME oxidation at a higher temperature e.g. 560 K for 1000 ppm of NO and 580 K for 2000 ppm of NO. NO clearly displays inhibiting effect on the oxidation kinetics of DME in the cool flame temperature regime. More interestingly, NO addition weakens the NTC behavior of DME (see Fig 1a-1c). The NTC behavior of DME completely disappears for 2000 ppm of NO. Unlike low temperatures, the addition of NO expedites the chemistry of DME at relatively high temperatures. For example, the complete fuel conversion of DME occurs at ~70 K lower for 2000 ppm of NO as opposed to neat DME. Our kinetic model accurately captures DME consumption with or without NO at lower temperatures; however, at the intermediate of 630 – 860 K, our model either overpredicts or underpredicts DME concentration depending upon the amount of NO added (see Fig 1a-1c). For major species (CO, CO₂, and H₂O), the model follows the experimental trend very well capturing the peak concentration satisfactorily. At low temperature (<600 K), our model suggests that neat DME decomposes mainly via the following route



The formed CH₂OCH₂O₂H further undergoes second O₂ addition to form O₂CH₂OCH₂O₂H which finally decomposes to ketohydroperoxides and OH radicals. In presence of NO, the decomposition channel of DME follows the following reaction pathways $\text{DME} \xrightarrow{+OH} \text{CH}_3\text{OCH}_2 \xrightarrow{+O_2} \text{CH}_3\text{OCH}_2\text{O}_2 \xrightarrow{+NO/\text{dissociation}} \text{CH}_3\text{OCH}_2\text{O}/2\text{CH}_2\text{O}+\text{OH}$. In presence of NO, CH₃OCH₂O₂ does not isomerize, and hence second O₂ addition does not happen. Rather CH₃OCH₂O₂ reacts with NO to form CH₃OCH₂O+NO₂ and CH₃OCH₂O dissociates to CH₃OCHO+H. The shift of the reaction pathways explains the weakening of cool flame chemistry of DME in presence of NO. As the temperature increases, the isomerization and dissociation pathways of CH₃OCH₂O₂ compete, and the dissociation pathway forming 2CH₂O+OH is more favorable at high temperatures.

Figure 2 shows the evolution of NO and NO₂ mole fraction profiles for the conditions specified in Fig. 1b-c. Experiments show the onset of NO consumption starting at ~550 K and ~570 K for 1000 ppm (Fig. 2a) and 2000 ppm (Fig. 2b) of NO, respectively. However, our model predicts the onset of NO consumption at somewhat lower temperatures, ~50 K lower for both cases. Despite this, the kinetic model was able to capture the experimental trend of NO consumption and NO₂ formation reasonably well.

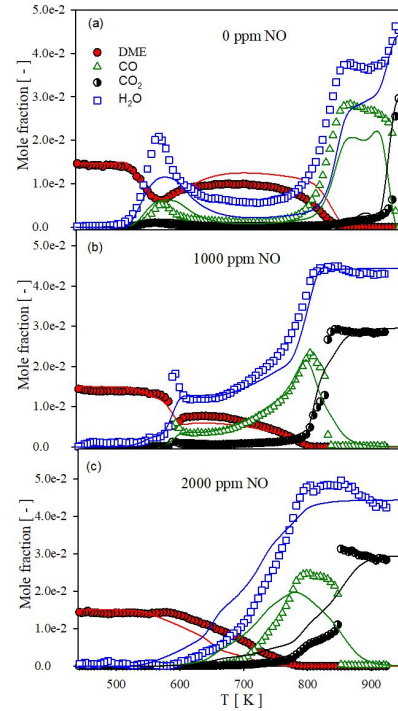


Figure 1: DME (OME₀)/O₂/Ar oxidation in a plug-flow reactor with different NO concentrations (0, 1000, and 2000 ppm) at $\phi = 0.8$ and 1 atm. Symbols: experimental data from Zhang et al. [15], Solid lines: modeling results from this work.

Interestingly, we made an observation that experiments reveal an early evolution of NO_2 before any fuel or NO was consumed (see Fig. 2a). This is not likely and may point to a high experimental uncertainty. Our model predictions for NO_2 are much closer to the experiments as compared to NO profiles. Figure 3 shows reaction flux analysis for “ NO - NO_2 looping” reactions. Note that only major pathways are shown. NO mainly reacts with RO_2 ($\text{CH}_3\text{OCH}_2\text{O}_2$) forming NO_2 and RO ($\text{CH}_3\text{OCH}_2\text{O}$) via $\text{CH}_3\text{OCH}_2\text{O}_2 + \text{NO} = \text{CH}_3\text{OCH}_2\text{O} + \text{NO}_2$ reaction.

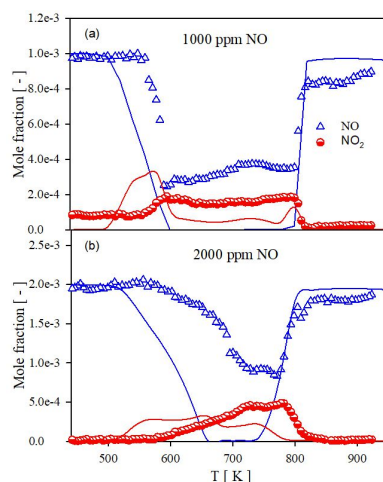


Figure 2: NO and NO_2 profiles during $\text{DME}/\text{O}_2/\text{Ar}$ oxidation in a flow reactor with different NO concentrations (a: 1000 ppm and b: 2000 ppm) at $\phi=0.8$ and 1 atm. Symbols: experimental data from Zhang *et al.* [15], Solid lines: the results of our modeling work.

This reaction is one of the most sensitive reactions for DME consumption (see Fig. 4). Under lean conditions, more HO_2 is available to react with NO forming NO_2 and OH . The formed NO_2 can further react with CH_3 radical to form a more stable product CH_3NO_2 (nitromethane). Furthermore, NO_2 can also react with fuel (DME) and the radicals like CH_3O and RO_2H ($\text{CH}_3\text{OCH}_2\text{O}_2\text{H}$) to give HONO to eventually produce NO via “ NO - NO_2 looping” reactions. The formed CH_3NO_2 further reacts with OH radical to give CH_2NO_2 which eventually dissociates to recycle back NO . During NO - NO_2 looping, reactive OH radicals are produced which expedite the oxidation kinetics of DME/NO at higher temperatures (>700 K). Figure 4 shows the most sensitive reactions for DME consumption in presence of 1000 ppm of NO . As can be seen, the most sensitive reactions are $\text{DME} + \text{NO}_2$ and $\text{DME} + \text{OH}$ radical reactions. The former reaction is a chain branching reaction producing HONO as one of the radicals that yields OH and NO radicals upon decomposition. Both of these radicals accelerate DME chemistry at high temperatures.

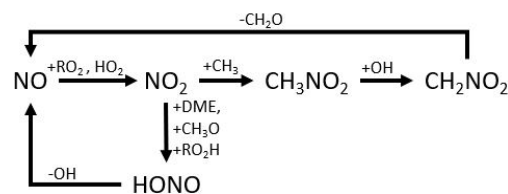


Figure 3: Integrated mass flux analysis based on N-atom at 700 K for 1000 ppm NO case during the oxidation of DME for the conditions shown in Figure 1b.

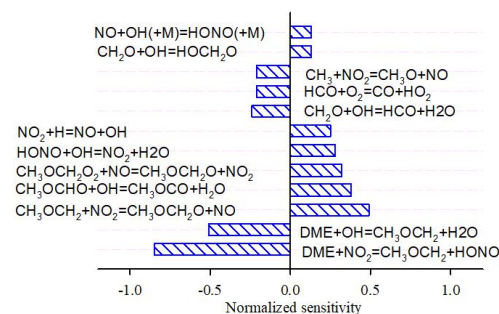


Figure 4: Reaction sensitivity analysis towards DME at 700 K for 1000 ppm NO case during DME oxidation as shown in Figure 1b.

NO_x chemical effect on DMM Oxidation

The modeling results are displayed in Figures 5 and 6 and compared with the experimental mole fractions (symbols). Again, the experimental data for DMM/NO oxidation were taken from Zhang *et al.* [15] who measured the species profiles in a plug-flow reactor at $\phi = 0.8$ and 1 atm over the temperature range of 400 – 1000 K with and without NO in the mixture. Unlike DME , DMM does not exhibit low temperature reactivity. As a result, no discernible NTC behavior was observed for neat DMM . This observation is in line with our earlier findings [17]. As can be seen in Fig. 5a, the actual onset of fuel oxidation occurs at ~ 660 showing slower reactivity than DME . Not much consumption of DMM was achieved up to 820 K. Beyond 820 K, DMM gets consumed rapidly. Adding 1000 ppm of NO , DMM gets consumed rapidly at ~ 160 K lower temperature than that of neat DMM . In addition, the weak NTC behavior was completely disappeared (see Fig. 5a and 5b). This is also true for the 2000 ppm NO case (Fig. 4c). For all cases, our model captures the fuel consumption profiles very closely within the experimental uncertainty of ± 20 K. For 2000 ppm NO case, the experimental data contradicts our modeling results. The onset of the reaction of $\text{DMM}/2000$ ppm NO is 40 K higher than $\text{DMM}/1000$ ppm NO , whereas the modeling does not discriminate the onset temperature between the two cases. For major species (H_2O , CO , and CO_2), the modeling results follow the experimental trend very well. They closely agree with the measurements and more so with NO doped cases as compared to neat DMM oxidation.

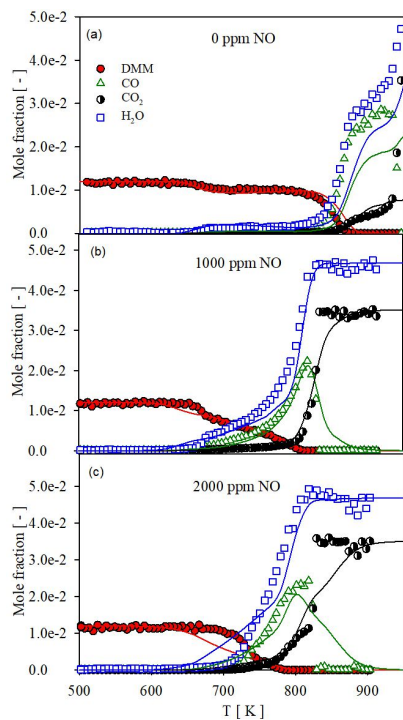
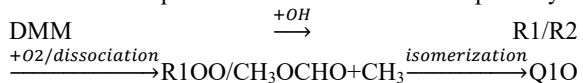


Figure 5: DMM (OME₁)/O₂/Ar oxidation in a flow reactor with varying concentrations of NO (0, 1000, and 2000 ppm) at $\phi = 0.8$ and 1 atm. Symbols and solid lines represent the experimental data from Zhang et al. [15] and model predictions of this work.

At 700 K, our model suggests that the consumption of DMM occurs via H-atom abstraction reactions by OH radical forming the terminal (CH₃OCH₂OCH₂, R1) and central (CH₃OCHOCH₃, R2) radicals. Both channels are found to be equally important for DMM consumption. DMM consumption occurs via the reaction pathways:



OH $\xrightarrow{dissociation}$ 1,3,5-trioxane + OH. At 700 K, only 13% of DMM is consumed when NO is not present while doping with 1000 ppm of NO, 42% of DMM gets consumed. In NO doped cases, DMM + NO₂ = R1 + HONO appears to be the topmost sensitive reaction (see Fig. 7 and 8). NO₂ accelerates the H-abstraction reaction by consuming DMM and forming 13% more R1 than R2 unlike the oxidation of neat DMM. Note that two primary hydrogen abstraction reactions consuming DMM show the opposite trend (see Fig. 8). The H-abstraction reaction at terminal C-atom enhances the reactivity while inhibiting the system reactivity at the central C-atom. Our results predict an earlier consumption of NO compared to the experimental data e.g. ~60 K and ~100 K lower temperature for 1000 ppm (Fig. 6a) and 2000 ppm (Fig. 6b) NO doped cases. At ~700 K, our model reveals a complete consumption of NO contrary to the experimental observation. Despite this, the model captured the experimental trend very well. Fig. 6 also

displays simulated NO₂ profiles. No experimental NO₂ profiles are available for comparison. Similar to the DME case (Fig. 2), the modeled NO₂ profiles peaked out before NO was completely consumed. However, the experimental data suggested otherwise (see Fig. 2) revealing that NO₂ concentration reaches a maximum at a temperature of maximum NO consumption. For these reasons, further improvement of the model is highly desirable to improve NO and NO₂ predictions.

We now briefly explore the important reaction pathways for “NO-NO₂ looping” in the oxidation kinetics of the DMM/NO chemical system. Figures 7 and 8 show the mass flux analysis based on the N-atom and DMM sensitivity analysis during oxidation kinetics of DMM in presence of 1000 ppm of NO, respectively.

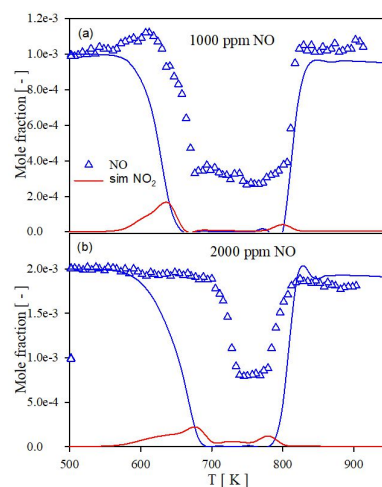


Figure 6: NO and NO₂ species profiles during DMM /O₂/Ar oxidation in a plug-flow reactor for varying NO concentrations (a: 1000 ppm and b: 2000 ppm) at $\phi = 0.8$ and 1 atm. Symbols represent measurement data from Zhang et al. [15] and the solid lines from this work.

Unlike the NO doped DME reaction system, the model suggests that the reactions of NO with DMM fuel-derived radicals (R1O₂ and RO₂) have minor contributions. NO mainly reacts with HO₂ and CH₃O₂ to produce NO₂ via NO + HO₂ = NO₂ + OH and NO + CH₃O₂ = NO₂ + CH₃O reactions.

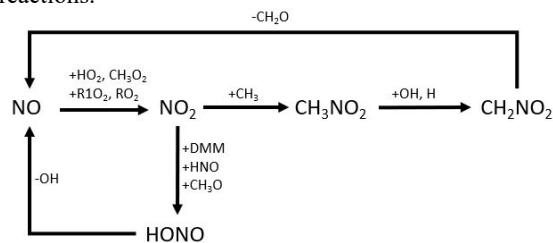


Figure 7: Integrated mass flux analysis based on N-atom carried out at $T = 700$ K, $\phi = 0.8$ and $P = 1$ atm for 1000 ppm NO/DMM case.

The formed NO_2 reacts with CH_3 radical forming CH_3NO_2 i.e backward reaction of $\text{CH}_3\text{NO}_2(+\text{M}) = \text{CH}_3 + \text{NO}_2(+\text{M})$. This is also one of the most sensitive reactions towards DMM (see Fig. 8). As discussed above, CH_3NO_2 eventually recycles back NO . NO_2 can react with fuel (DMM) and $\text{HNO}/\text{CH}_3\text{O}$ to yield HONO . The thermal dissociation of HONO recycles back NO producing reactive OH radicals which further enhances the reactivity of the system by increasing the radical pool.

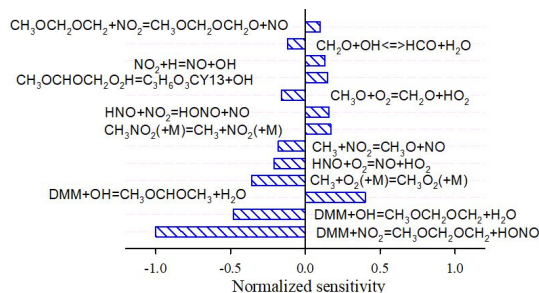


Figure 8: DMM sensitivity analysis carried out at $T = 700 \text{ K}$, $\phi = 0.8$ and $P = 1 \text{ atm}$ for 1000 ppm NO/DMM case.

Conclusions

We compiled a kinetic model based on our previous work to characterize the oxidation behaviour of dimethyl ether and dimethoxymethane with or without NO_x . We validated the robustness of our model against recently published plug-flow reactor data. Our results indicated that NO doping strongly affects the oxidation kinetics of both fuels. The sensitizing effects of NO_x on DME and DMM oxidation kinetics are severe. NO_x addition dramatically altered the shape of the fuel consumption profiles. The addition of NO in both fuels enhanced the reactivity of the system by moving the onset temperature of complete fuel oxidation at a lower temperature. However, NO was found to severely inhibit the reactivity of DME in the cool flame temperature regime. The inhibiting of the NTC behavior is mainly due to the competition of $\text{CH}_3\text{OCH}_2\text{O}_2$ radical reaction with NO ($\text{CH}_3\text{OCH}_2\text{O}_2 + \text{NO} = \text{CH}_3\text{OCH}_2\text{O} + \text{NO}_2$) and the isomerization ($\text{CH}_2\text{OCH}_2\text{O}_2\text{H}/\text{dissociation} = (\text{CH}_2\text{O} + \text{CH}_2\text{O} + \text{OH})$) channels. Unlike DME, DMM does not exhibit a strong NTC behavior. The weak NTC behavior of DMM is completely suppressed in presence of NO . For both fuels, the reaction of NO_2 with the parent fuel appears to be the most sensitive ($\text{DME}/\text{DMM} + \text{NO}_2 = \text{CH}_3\text{OCH}_2/\text{CH}_3\text{OCH}_2\text{OCH}_2 + \text{HONO}$). However, some discrepancies between the modeling and experimental results were observed. Therefore, more experimental studies focusing on NO_x interaction with DME and DMM fuels system are needed. Such studies will improve the current mechanistic understanding for DME and DMM oxidation in presence of NO_x . Moreover, these efforts will form the basis of model development of larger ethers- NO_x systems.

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