The influence of dimethoxy methane (DMM)/dimethyl carbonate (DMC) addition on premixed ethane/oxygen/argon flame

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Abstract: Two series of laminar premixed flames fueled by ethane-oxygenate-argon mixtures, in which ethane was incrementally replaced with either dimethoxy methane (DMM) or dimethyl carbonate (DMC) by mole fractions of 25%, 50% and 75%, were investigated at a fixed carbon to oxygen ratio (C/O) of 0.50 and a pressure of 40 mbar. Mole fractions for flame species were obtained by employing molecular-beam mass spectrometry with synchrotron vacuum ultraviolet light for ionization. A detailed kinetic model including the chemistry of ethane, DMM and DMC was constructed and tested against the flame measurements. The effects of the addition of oxygenates to the species pool were studied, especially considering peak mole fractions of harmful emissions and relevant intermediates. The results indicate that the variation behaviors are mainly related to “volume effects” without strong chemical interactions between the fuel pairs. DMM and DMC show comparable performance in inhibiting soot precursors with the same addition amount. Formaldehyde is a major oxygenated emission in both flame series, almost linearly increasing with the addition of DMM or DMC, which is the consequence of the structural and kinetic characteristics of both oxygenates.

Keywords: Dimethoxy methane (DMM); Dimethyl carbonate (DMC); Flame intermediates; Blended fuel; Mass spectrometry

1. Introduction

As renewable non-fossil fuels, oxygenated hydrocarbons are believed to produce less soot when compared to hydrocarbons under equivalent conditions [1, 2]. Because oxygenated fuels are commonly used as fuel additives, their soot-inhibition ability is usually influenced by both the chemistry of the base hydrocarbon fuels and the oxygenated additives as well as their chemical interactions. Considerable attention has been paid to this research field with the base fuel ranging from simple compounds like ethane [3], ethylene[4, 5], propene [6, 7] and 1,3-butadiene [8, 9], to larger ones such as heptane[10], benzene [11] and practical diesel fuels [12, 13]. It was reported in several engine studies [12, 13] that only the oxygen mass fraction of the fuel mixture affects the extent of soot reduction. However other considerable studies suggested that the molecular structures of added oxygenates [1, 6, 14] also influence the extent of soot reduction. Other factors such as the initial C/O ratio [4, 5, 11] and the content of C-C bonds in fuel mixtures [15] were also suggested to be relevant factors. Unfortunately, the benefit of such a soot reduction by oxygenated additives is achieved at the cost of an undesired and increased emission of toxic oxygenates like aldehydes and ketones [2, 6]. The emissions are certainly the results of interactions among the whole reaction networks, which could be adjusted by altering the composition of fuel mixtures. A good understanding of the detailed combustion chemistry of newly proposed oxygenated fuels and blended fuels is therefore of great interest and is crucial in achieving a balanced soot and oxygenated emission [2].

In this study, two promising oxygenated additives, dimethoxy methane ($\text{CH}_3\text{OCH}_2\text{OCH}_3$, DMM), and dimethyl carbonate [$\text{CH}_3\text{OC}(=\text{O})\text{OCH}_3$, DMC] were investigated, both being non-toxic and highly miscible with diesel fuels. Carbon-carbon (C-C) bonds are absent from the molecular

structures of DMM and DMC. Their great soot-reduction potential can be expected due to their high mass fractions of oxygen (0.42 for DMM and 0.53 for DMC). The combustion kinetics of both DMM and DMC have been investigated in several previous studies [4, 5, 10, 16-19], however, the interactions with hydrocarbon fuels need to be further revealed from a perspective of kinetics. Ethane (C_2H_6) was chosen as the base fuel enabling the investigation of the influences of C-C bonds to the reaction patterns of DMM and DMC. In this study, flames containing 0, 25, 50 and 75% DMM (or DMC) with a fixed C/O ratio of 0.50 were measured with photoionization mass spectrometry (PIMS). The variation range of the fuel composition is wide enough so that the gradual variation trends of species concentrations can be well captured. A kinetic model was constructed and validated against the experimental results. The experimental and modeling efforts were combined to elucidate the progressive changes in the species pool and the possible interactions between the base fuel and the respective oxygenated additives. The influence of the molecular structures of the oxygenated additives with regards to toxic emissions will also be discussed.

2. Experimental Method

The experimental work was performed at the Advanced Light Source (ALS) at the Lawrence Berkeley National Laboratory. The apparatus includes a McKenna-type burner, a molecular beam sampling system and a reflectron time-of-flight mass spectrometer (TOFMS). The synchrotron vacuum ultraviolet (VUV) light is used for ionization. Both are described in detail elsewhere [20, 21]. A total of eight flames, including a neat DMM flame, a base ethane flame and the blended series, were investigated in this study. Ethane in the base flame was replaced incrementally, from 25 mol% up to 75 mol%, by either DMM or DMC with the C/O ratio fixed at 0.50. For all flames the total

volume flow rate was kept at 4 standard liters per minute (SLM) with an argon dilution ratio of 25%. The pressure was kept at 40 mbar (with an uncertainty of $\pm 1\%$) to maximize the flame thickness and stand-off distance while maintaining flame stability. The detailed flame conditions are provided in **Table 1**. The gas flows (O_2 , Ar and C_2H_6) were controlled separately by mass flow controllers, while the flow of liquid DMM or DMC was metered by a syringe pump before entering a vaporizer. Errors for all flow rates were estimated within 2% of the target values. Flame gases were sampled along the axis of the flames by a quartz cone of 0.25 mm orifice diameter and cone angle of 40° . The molecular beam from the sampling system was crossed by the dispersed VUV light from the monochromator and photo-ions were collected and mass-analyzed with the TOFMS which provides a mass resolution of $m/\Delta m$ up to 400. The integrated ion intensities for a specific mass were normalized to the photon flux, and then plotted as a function of the photon energy or distance from the burner surface, which yielded photoionization efficiency (PIE) or mole fraction profiles, respectively. Flame temperature profiles were measured using laser-induced fluorescence (LIF) from OH, as described by McIlroy *et al.* [22]. The uncertainty of the temperature measurement was estimated as ± 100 K [23]. The temperature at the burner surface (0 mm) could not be experimentally determined and was estimated to be 500 K. When performing model simulations, we followed the practice of shifting the measured temperature profiles by 1 mm downstream to compensate the probe effect [24].

The uncertainties for species mole fractions were estimated according to our recent study [19] of laminar premixed DMC flames under similar conditions. For major species the uncertainty factor (UF) is estimated as 1.2, increasing to 1.3 within the reaction zone (For the mole fraction x of a certain species, the uncertainty range is between the upper limit of $x \cdot UF$ and the lower limit of

x/UF). For stable intermediates with measured photon ionization cross sections (PICSs), the UF is within 1.7, and for radicals or species with estimated PICSs, the factors can be as large as 3-4. The estimated UF s of the peak mole fractions for separate intermediates are provided in **Table S1** together with the PICS and mass discrimination (MD) factors used in the data evaluation procedure. The measured mole fractions less than 1 mm away from the burner are not provided due to relatively severe sampling effects in this region [25].

All measured flame structures including temperature and species mole fraction profiles are provided in the *Supplemental material*.

Table 1

Detailed flame conditions for all neat and blended flames

No.	Fuel composition	Pressure (mbar)	Volume flow rate (SLM)					C/O ratio	Equivalence ratio (ϕ)
			DMM	DMC	C ₂ H ₆	O ₂	Ar		
1	neat C ₂ H ₆	40.0	0.00	0.00	1.00	2.01	1.00	0.50	1.74
2	neat DMM	40.0	1.00	0.00	0.00	2.00	1.00	0.50	2.00
3	25%DMM +75% C ₂ H ₆	40.0	0.25	0.00	0.75	2.00	1.00	0.50	1.81
4	50%DMM +50% C ₂ H ₆	40.0	0.50	0.00	0.50	2.00	1.00	0.50	1.88
5	75%DMM +25% C ₂ H ₆	40.0	0.75	0.00	0.25	2.00	1.00	0.50	1.94
6	25%DMC +75% C ₂ H ₆	40.0	0.00	0.26	0.78	1.96	1.00	0.50	1.79
7	50%DMC +50% C ₂ H ₆	40.0	0.00	0.55	0.55	1.91	1.00	0.50	1.87
8	75%DMC +25% C ₂ H ₆	40.0	0.00	0.86	0.29	1.86	1.00	0.50	1.93

3. Kinetic modeling

A detailed kinetic model was constructed by integrating the chemical kinetics of C_2H_6 , DMM and DMC. The extensively validated C_0 - C_4 mechanism AramcoMech1.3 [26] was employed as the core mechanism which includes reactions of crucial oxygenated intermediates in DMM and DMC combustion. The C_5 - C_6 reactions, including benzene (C_6H_6) formation pathways, were taken from a cyclohexane mechanism by Li *et al.* [27] in which the pressure-dependent rate coefficients of key reactions like the recombination of C_3H_3 , conversions among C_3 species (C_3H_4 , C_3H_3 and C_3H_2) and C_4+C_2 reactions were extracted from high-level theoretical works [28-31]. Besides, according to further model analysis, reactions related to the species C_3H_2 from [27] were added to the model and rate coefficients for the reaction pair of $C_3H_3+H=C_3H_4$ -p/ C_3H_4 -a were updated with the calculations by Miller *et al.* [28]. The DMM sub-mechanism was taken from the kinetic model proposed by Glaude *et al.* [17], and the DMC sub-mechanism was originated from our recent study [19].

We ensured the consistency of thermochemical properties and transport data for all species before merging the abovementioned sub-mechanisms. 283 species and 1715 reactions are included in the entire model, which is provided in the [Supplemental Material](#).

The simulations were performed using the Premixed code of Chemkin Pro software [32]. The measured temperature profiles were taken as input parameters. The multi-component transport and thermal diffusion were considered in the calculations.

4. Results and discussion

4.1 Model validation

The performance of the model was tested against all measured flame structures in the present study and the neat DMC flame reported in Ref. [19]. The agreements between experimental and simulated species mole fractions are satisfactory for all investigated flames. For examples, the major species [CO_2 , CO , H_2O , H_2 , Ar , O_2 , C_2H_6 , DMM (or DMC)] mole fraction profiles in the blended flames with 50% DMM (or DMC) addition, including measurements and simulations, are

presented in **Fig. S1** in the *Supplemental material*. It can be noted that with the same addition amount of DMM and DMC, CO_2 is produced at a much faster pace in the DMC blended flame. Simulated mole fraction distributions for main intermediates are compared with the corresponding measurements in these two blended flames with 50% DMM (or DMC) addition, as demonstrated in **Fig. 1**. Both the shapes and the concentrations can be well captured by the current model, with the estimated uncertainties taken into account. Good agreement between experiments and simulations is also achieved in the neat flames (C_2H_6 and DMM), as presented in **Figs. S1-S2**. The validated model was then used for the analysis of reaction pathways and further discussions of possible interactions within the species pool and reaction networks.

Fig. 1. Comparison between experimental and simulated mole fractions of main intermediates in (a) the 50% C_2H_6 +50%DMM flame and (b) the 50% C_2H_6 +50%DMC flame.

4.2 Combustion characteristics and fuel consumption

Insights into the changing species pool and the reaction networks can be gained through the

combined experimental and modeling efforts. A previous study [23] suggested that mechanistic conclusions were unlikely to change with an experimental uncertainty in temperature as large as 200 K in flame conditions. The measured temperatures (see **Fig. S3** in the *Supplemental Material*) in the different investigated flames are similar at the same positions, especially in the reaction zone where the intermediates are formed and depleted. Therefore the influences of temperature difference are excluded in the following discussion.

To have a clear understanding of the reaction patterns, schemes of the reaction network for the neat C₂H₆ and DMM flames are established in **Fig. 2** based on the rate of production (ROP) analysis of specific species by integrating the ROP coefficients along the entire flame range. The reaction network for DMC under similar conditions was discussed in our previous study [19], which is provided as **Fig. S4** in the *Supplemental material*. For C₂H₆ flame, the fuel is completely consumed through hydrogen abstractions, and the subsequent dehydrogenation process C₂H₅ → C₂H₄ → C₂H₃ → C₂H₂ is the dominating pathway of the C₂ species. Recombination with C₁ species and oxidation pathways are also important and yield larger hydrocarbons and oxygenated intermediates, respectively. For DMM and DMC flames, hydrogen abstractions dominant the fuel consumption, while the unimolecular decompositions, including bond fissions and eliminations, also have remarkable (up to 40%) contributions. The most important unimolecular decomposition pathway for DMM is the one yielding methanol (CH₃OH), formyl (HCO) and methyl (CH₃), which is actually a two-step process, *i.e.* DMM produces CH₃OH and CH₃OCH through a three-membered H atom transfer process, and at a much faster pace the reactive carbene CH₃OCH decomposes to HCO and CH₃. While for DMC the CO₂ elimination through a four-membered transition state is the major unimolecular pathway. The oxygenated intermediates, methyl formate (CH₃OCHO) and dimethyl ether (CH₃OCH₃, DME) are produced in the primary reactions of DMM and DMC, respectively.

ROP analysis of the fuel consumption was also performed in the entire range of the blended flames. According to relevant ROP analyzed results, when progressively increasing the addition amount of DMM (or DMC), no obvious changes can be observed in the decomposition pathways of

individual fuels, which are still dominated by the hydrogen abstractions as mentioned above. This indicates that the fuel consumptions are barely affected by the fuel composition in the studied flames.

Fig. 2. Reaction pathways based on ROP analysis in the entire flame range for (a) C_2H_6 and (b) DMM in their neat fuel-rich premixed flames. The numbers are percent contributions to the consumption of the species on the source side of the arrow.

4.3 Intermediates and harmful emissions

The experimental measurements of the chemical compositions for separate flames can provide an overview of the species pool. Most of the detected species are shared in all investigated flames and no other species were observed in the blended series beyond the combined species pools of individual neat flames. However, the concentrations for specific species vary in a wide range for different flames. **Figure 3** summarizes the experimental and simulated peak mole fractions for several crucial intermediates including methyl (CH_3), acetylene (C_2H_2), ethylene (C_2H_4), propargyl (C_3H_3), C_6H_6 , formaldehyde (CH_2O), acetaldehyde (CH_3CHO), methyl formate (CH_3OCHO) and dimethyl ether (CH_3OCH_3). For each of the above species in the two flame series blended respectively with DMM and DMC, the mole fraction variation trends are compared. All the model predictions are within the experimental error limits.

Fig. 3. Peak mole fractions (multiplied by 10^5) of several crucial intermediates in different blended flames. *Symbols with error bars*: measurements with corresponding estimated uncertainties; *Bars*: predictions. The lines connecting the bars only serve as guides of the variation trends.

As shown in **Fig.3(a)** the concentrations of CH_3 almost stay constant in the different flames, which could be affiliated to the numerous reactions involving CH_3 . The ROP analysis reveals that in the neat C_2H_6 flame, CH_3 formation is dominated by the $\text{C}_2\text{H}_5 + \text{H}$ reaction (see **Fig. 1**), while the contributions of the β -scissions of CH_3OCH_2 and CH_3OCO radicals become obvious when respectively adding DMM and DMC. Besides the oxidation by O and OH, the self-recombination of CH_3 plays a role in its consumption in the blended flames. For all C_2 and larger hydrocarbons, obvious declining trends can be observed in the peak mole fractions when increasing the portion of DMM (or DMC). For C_2H_2 and C_2H_4 , with significant levels reaching the magnitude of 10^4 ppm, the peak concentrations almost linearly decrease. To facilitate the discussion, a definition of “volume effects” is provided first. Assuming that DMM in the blended series is replaced by argon with the C/O ratio kept at 0.50, chemical structures of the argon diluent ethane flame series are simulated with temperature profiles in corresponding blended flames. The mole fraction distributions of C_2H_4 in these flames are presented in **Fig. 4** with the peak mole fractions shown in the inset. As a reference, simulated C_2H_4 peak mole fractions in DMM blended flame series are also

presented. It can be noted that C_2H_4 peak mole fraction variations in the two flame series almost coincide. Therefore when adding DMM to the base ethane flame, DMM acts almost like a dilution gas, leading to the reduced level of C_2H_4 . Such diluent effects of DMM in respect of C_2H_4 concentration is defined as “volume effects” in the present study. By conducting similar model analysis, it is proven that linear declines of C_2 intermediates in both DMM and DMC blended series are resulted from “volume effects”. That is because C_2 species can hardly be directly formed through decomposition of DMM (or DMC) due to the absence of carbon-carbon (C-C) bonds in both oxygenates, but can be easily formed through the above-mentioned dehydrogenation process of C_2H_6 .

Fig.4. Model predicting C_2H_4 mole fraction profiles in neat argon diluent ethane flames, for each of which the initial ethane concentration, C/O ratio and the temperature profile are kept the same with those of the corresponding DMM blended flame. Peak mole fractions in the argon diluent and DMM blended series are shown in the inset.

The self-recombination of C_3H_3 , a resonantly stabilized radical, has been well established as a key route of benzene formation in combustion processes of most acyclic hydrocarbons [28]. ROP analysis was performed for C_3H_3 in each flame, and the results for the C_2H_6 /DMM blends are shown in **Fig. 5** while those for the C_2H_6 /DMC series are provided in **Fig. S5** in the [Supplemental Material](#). In all flames, the recombination of C_2H_2 with methylene radicals [CH_2 and $CH_2(s)$] is the principal source of C_3H_3 which can combine with CH_2 to produce larger hydrocarbons, otherwise break down through hydrogen abstractions by OH or oxidization by O. When progressively adding DMM (or DMC), the relative importance of recombination is reduced while the abstraction and oxidation reactions contribute more to C_3H_3 consumption, which is consistent with the enhanced

OH concentrations, as shown in **Fig. S6**. In addition, plenty of O atoms would be introduced to the mixtures when adding the oxygen-containing compounds. As a consequence, C_6H_6 was only detected in the base C_2H_6 flame and the blended one with 25% DMM addition, as demonstrated in **Fig. 3(e)**. The modeled peak concentration of C_6H_6 drops under the ppm magnitude when about 50% ethane is replaced by DMM and DMC, respectively. The approximately quadratic decline might be attributed to the linear decrease of C_3H_3 , whose recombination contribute to the majority of C_6H_6 formation.

Fig. 5. Normalized ROP analysis of C_3H_3 in the C_2H_6 /DMM blended flame series.

The peak concentrations of all the mentioned unsaturated hydrocarbons show similar decreasing trends in the DMM and DMC blended series. This suggests that the same extent of reduction can be achieved with the equal addition amount (by mole fraction) of DMM and DMC. Recognizing that two and three oxygen atoms are imbedded in the molecular structures of DMM and DMC, respectively, the oxygen atoms in DMM are therefore more efficiently utilized in reducing the soot/PAH formation. In the practical application, oxygenated additives are usually blended to the diesel fuel by liquid volume fraction. With the same liquid-volume addition, the molar amount of DMM and DMC is almost identical (113:119) with the basic physical properties for the two oxygenates (DMM: 0.856 g/cm³, 76.10 g/mol; DMC: 1.069 g/cm³, 90.07 g/mol) taken into consideration. Furthermore, with the higher heat value (1.702 MJ/mol for DMM and 1.215 MJ/mol for DMC), DMM might be a better choice for practical use.

The increasing emission of oxygenated pollutants is an unavoidable problem when putting oxygenated fuels to practical use. Two simple aldehydes, formaldehyde (CH_2O) and acetaldehyde (CH_3CHO) were detected in all flames, whose peak mole fractions are presented in **Fig. 3 (f)-(g)**. The extremely high concentrations (over 10^4 ppm) of CH_2O in the blended flames can be explained by the reaction patterns of DMM and DMC. As mentioned above, the hydrogen abstractions dominate the consumption of DMM and DMC in flame conditions, and when the primary hydrogen atoms in DMM and DMC are abstracted, the corresponding fuel radicals, $\text{CH}_3\text{OCH}_2\text{OCH}_2$ and $\text{CH}_3\text{OC}(=\text{O})\text{OCH}_2$ subsequently break down through β -scissions yielding CH_2O . The peak mole fractions of CH_2O in both blended series linearly increase with the portion of DMM (or DMC), at a faster pace in the DMM series. This behavior can be traced back to the $\text{C}(=\text{O})$ imbedded DMC that cannot participate in the formation of CH_2O . As a consequence the peak mole fraction of CH_3CHO decreases when increasing the amount of DMM (or DMC). According to the results of relevant ROP analysis, the oxidation of C_2H_5 and isomerization of ethenol ($\text{C}_2\text{H}_3\text{OH}$) are the two principal sources of CH_3CHO formation and $\text{C}_2\text{H}_3\text{OH}$ originates nearly exclusively from the oxidation of C_2H_4 by OH according to relevant ROP-analyzed results. Both C_2H_5 and C_2H_4 are crucial intermediates in the consumption paths of C_2H_6 . Furthermore, because of the absence of C-C bonds in the molecular structure of DMM and DMC, no fuel-related reactions directly contribute to the formation of CH_3CHO . Therefore the reduction of CH_3CHO concentrations can be mainly attributed to the lower initial content of C_2H_6 in the fuel mixture. Two oxygenated intermediates, CH_3OCHO and CH_3OCH_3 , are abundant in DMM and DMC blended series, respectively. Their peak mole fractions increase linearly with the amount of added oxygenates. This trend can be traced back to the reaction pathways of the two oxygenates. The radical $\text{CH}_3\text{OCHOCH}_3$, formed from the secondary H atom abstracted from DMM, breaks down through the energy-favored β -scission, simultaneously producing CH_3OCHO and CH_3 . In the case of DMC, CH_3OCH_3 can be directly released from the CO_2 elimination ($\text{CH}_3\text{OC}(=\text{O})\text{OCH}_3 = \text{CH}_3\text{OCH}_3 + \text{CO}_2$). These two species were not observed in the neat C_2H_6 flame without direct formation pathways. Influences of C_2H_6 initial

concentration on CH_3OCHO and CH_3OCH_3 peak mole fractions can also be attributed to “volume effects” as mentioned previously. To be more general, when a specific intermediate is predominantly produced from the consumption of only one component in a binary hydrocarbon/oxygenate fuel mixture, the other fuel component acts almost like a dilution, reactions of which could have negligible effects in respect of that intermediate.

It can be noted in **Table 1** that in the present experiments at the fixed C/O ratio of 0.50, because of the altered fuel composition, equivalence ratio covered a range of 1.74-1.94 and 1.74~1.93 in the DMM and DMC series, respectively. Therefore concerns might arise that the observed variations might be attributed to the change in equivalence ratios, rather than the incrementally changed fuel composition. To address this issue, model simulations were performed for both blended flame series at the fixed equivalence ratios of 1.84, which was actually the mid-value of the equivalence ratio variation ranges so the similarity of the flames in the same series could be ensured. For examples, the peak mole fractions of C_2H_2 and CH_2O in the DMM series predicted by the model are illustrated in **Fig. 6**. Corresponding peak mole fractions at the fixed C/O ratio of 0.50 (the conditions of the current study) are also presented as a reference. According to the results, the similar linear decrease in C_2H_2 and increase in CH_2O concentrations can be captured when either parameter is fixed. This behavior indicates that the observed variation patterns of the species concentrations are indeed brought by the blending.

Fig. 6. Model predicting peak mole fractions in the C_2H_6 /DMM blended flame series at fixed ϕ of 1.84 and fixed C/O of 0.50.

5. Conclusion

Chemical structures of two series of ethane-DMM (or DMC) blended flames with incrementally varying fuel composition were measured with the photoionization molecular beam mass spectrometry. A kinetic model was constructed and tested with the current measurements. The validated model and the experimental results were then used to explore the possible interactions among the radical pool and reaction networks, with focus on the harmful emissions. Both oxygenates (DMM and DMC) are effective in reducing unsaturated hydrocarbons because C-C bonds are absent from their molecular structures. With equal amount (by mole fraction) of DMM and DMC addition, the unsaturated hydrocarbons are reduced to almost the same extent. As two and three oxygen atoms are imbedded in DMM and DMC, respectively, DMM could be the better choice as a soot/PAH inhibitor in the perspective of O atoms usage efficiency. Both oxygenated fuels enhance the formation of CH_2O , whereas DMM has a more remarkable effect than DMC. This could be attributed to the fact that CH_2O can be directly yielded from the β -scissions of the fuel radicals [$CH_3OCH_2OCH_2$ and $CH_3OC(=O)OCH_2$] formed through hydrogen abstractions. The observed linear variations in species concentrations when progressively increasing the addition

amount of either oxygenate are mainly the result of “volume effects”, instead of strong chemical interactions.

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Figure captions:

Fig.1. Comparison between experimental and simulated mole fractions of main intermediates in (a) the 50% C_2H_6 +50%DMM flame and (b) the 50% C_2H_6 +50%DMC flame.

Fig. 2. Reaction pathways based on ROP analysis in the entire flame range for (a) C_2H_6 and (b) DMM in their neat fuel-rich premixed flames. The numbers are percent contributions to the consumption of the species on the source side of the arrow.

Fig. 3. Peak mole fractions (multiplied by 10^5) of several crucial intermediates in different blended flames. *Symbols with error bars*: measurements with corresponding estimated uncertainties; *Bars*: predictions. The lines connecting the bars only serve as guides of the variation trends.

Fig.4. Model predicting C_2H_4 mole fraction profiles in neat argon diluent ethane flames, for each of which the initial ethane concentration, C/O ratio and the temperature profile is kept the same with that of the corresponding DMM blended flame. Peak mole fractions in the argon diluent and DMM blended series are shown in the inset.

Fig.5. Normalized ROP analysis of C_3H_3 in the C_2H_6 /DMM blended flame series.

Fig.6. Model predicting peak mole fractions in the C_2H_6 /DMM blended flame series at fixed ϕ of 1.84 and fixed C/O of 0.50.