

Effects of dimethyl ether on n-butane oxidation



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HIGHLIGHTS

- ▶ Effects of DME addition to n-butane oxidation were studied.
- ▶ DME was found to decrease the formations of CO, aromatic species and PAHs.
- ▶ DME addition increased the formations of formaldehyde and acetaldehyde.
- ▶ Effects of equivalence ratio were investigated in fuel-rich conditions.
- ▶ Increasing equivalence ratio increased the formations of aromatic and PAH species.

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ABSTRACT

Dimethyl ether (DME) is the simplest ether and it is used as an alternative fuel or fuel additive to reduce toxic emissions from combustion processes. The effects of DME on n-butane oxidation were investigated for two different concentrations of DME in the fuel mixture (i.e., 20% and 50%) and two different fuel-rich equivalence ratios (i.e., 2.6 and 3.0) using detailed chemical kinetic modeling. Reactor model was selected as atmospheric-pressure, adiabatic, tubular reactor, operated under laminar flow conditions. The concentration profiles of major, minor, and trace species were obtained for n-butane/DME/oxygen/argon at six different reactor inlet temperatures, and the results were compared with those attained for pure n-butane oxidation case (n-butane/oxygen/argon). Dimethyl ether addition decreased formations of various toxic species such as carbon monoxide, aromatic species, and polycyclic aromatic hydrocarbons, while it increased the formations of formaldehyde and acetaldehyde. Increasing equivalence ratio increased the formations of carbon monoxide, methane, aromatic species, and polycyclic aromatic hydrocarbons, while its effects on formaldehyde and acetaldehyde were not pronounced under the conditions studied.

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1. Introduction

One of the major sources of current environmental pollution is the toxic air pollutants released from combustion and oxidation processes utilized in manufacturing, transportation, and power generation industries. Formations of these hazardous compounds are related to the oxidation chemistries of fuels and process conditions. Theoretical modeling is one of the most widely used methods for investigation of oxidation processes and formations of oxidation products. The conversions of the reactants into different products are described by detailed chemical kinetic modeling at molecular level.

Fuels utilized currently are almost totally composed of hydrocarbons. n-Butane (C₄H₁₀), one type of hydrocarbon fuel, is an alkane that is widely used in internal combustion engines,

industrial burners, and residential heating, and is a main component of LPG (liquefied petroleum gas). Although it is known to be a cleaner fuel producing lower emissions compared to gasoline and diesel; there are still some types of emissions such as CO, polycyclic aromatic hydrocarbons (PAHs), and soot, associated with the usage of n-butane, especially at fuel-rich conditions. These compounds are known to be toxic or carcinogenic [1].

The addition of oxygenated fuel-additives to hydrocarbon fuels is one of the methods applied in reduction of hazardous emissions from oxidation processes. Dimethyl ether (DME, CH₃OCH₃), one of these oxygenated additives, is the simplest ether with an oxygen atom in its structure. It does not contain any C–C bonds and has the lowest C/H ratio after methane. Its handling characteristics are similar to butane and propane.

DME can be produced from variety of sources such as natural gas, coal, and biomass. Worldwide DME production capacity and actual market use have been reported to be about 10 million metric tons per year and 3 million metric tons per year, respectively [2]. China is the leader country in DME production and use. Currently,

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more than 90% of DME produced in China is used as a LPG blend stock for domestic uses. Other leading markets for DME are; transportation fuel, fuel for power generation, and chemical feedstock for olefins and gasoline [2,3].

Marchionna et al. [4] have investigated the potential application of DME as a substitute fuel in domestic appliances commonly fed with LPG. Five cooking hobs with three different types of burners were used in the experiments. The results showed that while the use of pure DME requires making a few changes to the burners, 15–20 vol% DME in a mixture of DME/LPG (LPG: C3/C4 ratio of 65/35) could be utilized without any modification of standard equipment used for pure LPG. The positive effects of DME addition to LPG were also observed with respect to CO and NO emissions.

CO and NO emissions from DME and conventional utility fuels propane and n-butane were also studied in laminar premixed flames on the basis of constant mass flow (0.3 g/min), constant C-atom flow normalized to n-butane, and constant energy release rate of 100 J/s over a wide range of equivalence ratios [5]. The results indicated that while lower CO emission was obtained from DME fuel on all three bases, NO production was generally less than or similar to that of propane and n-butane.

Due to its superior physical and chemical properties such as high cetane number (>55), low boiling point, low auto-ignition temperature, and simultaneous reductions in NO_x and smoke emissions, DME has been considered as a potential diesel engine fuel. Pure diesel and DME were used to study exhaust CO, NO_x, total hydrocarbon (THC), smoke, and formaldehyde emissions from a

four-stroke, two-cylinder, direct injection diesel engine at two engine speeds (1400 rpm and 1870 rpm) [6]. CO and NO_x emissions were decreased by 59% and 45.2% at 1400 rpm, and 23.7% and 57.9% at 1870 rpm, respectively when DME was used as a fuel. The THC emissions from DME fuel were close to that from diesel fuel. Smoke emission was almost zero for DME under the experimental conditions investigated. However, formaldehyde emission with DME was slightly higher than that with diesel fuel. Xinling and Zhen [7] have also reported substantial reductions in THC (40.1%) and NO_x (48.2%) emissions from a 6-cylinder, medium-duty, direct injection, turbocharged diesel engine for DME compared with diesel fuel.

The performance, emissions characteristics, and combustion stability of a single cylinder compression ignition (CI) engine operated with n-butane blended DME (0–40% n-butane by mass) and diesel fuels were studied at 1500 rpm [8]. The combustion stability of the blended fuel was better in comparison to diesel fuel, and stable engine operation was reported for a wide range of engine loads up to 30% n-butane by mass in n-butane/DME blend. The engine power output and fuel consumption were improved with n-butane/DME blend. CO and THC emissions were increased at low engine loads when fuel blend was used. Soot and NO_x emissions were similar for all blends. However, NO_x emissions for blended fuels were lower than those for diesel fuel.

The major drawbacks of DME as an alternative fuel for internal combustion engines compared with petroleum based conventional fuels are; its low enthalpy of combustion due to about 35% oxygen

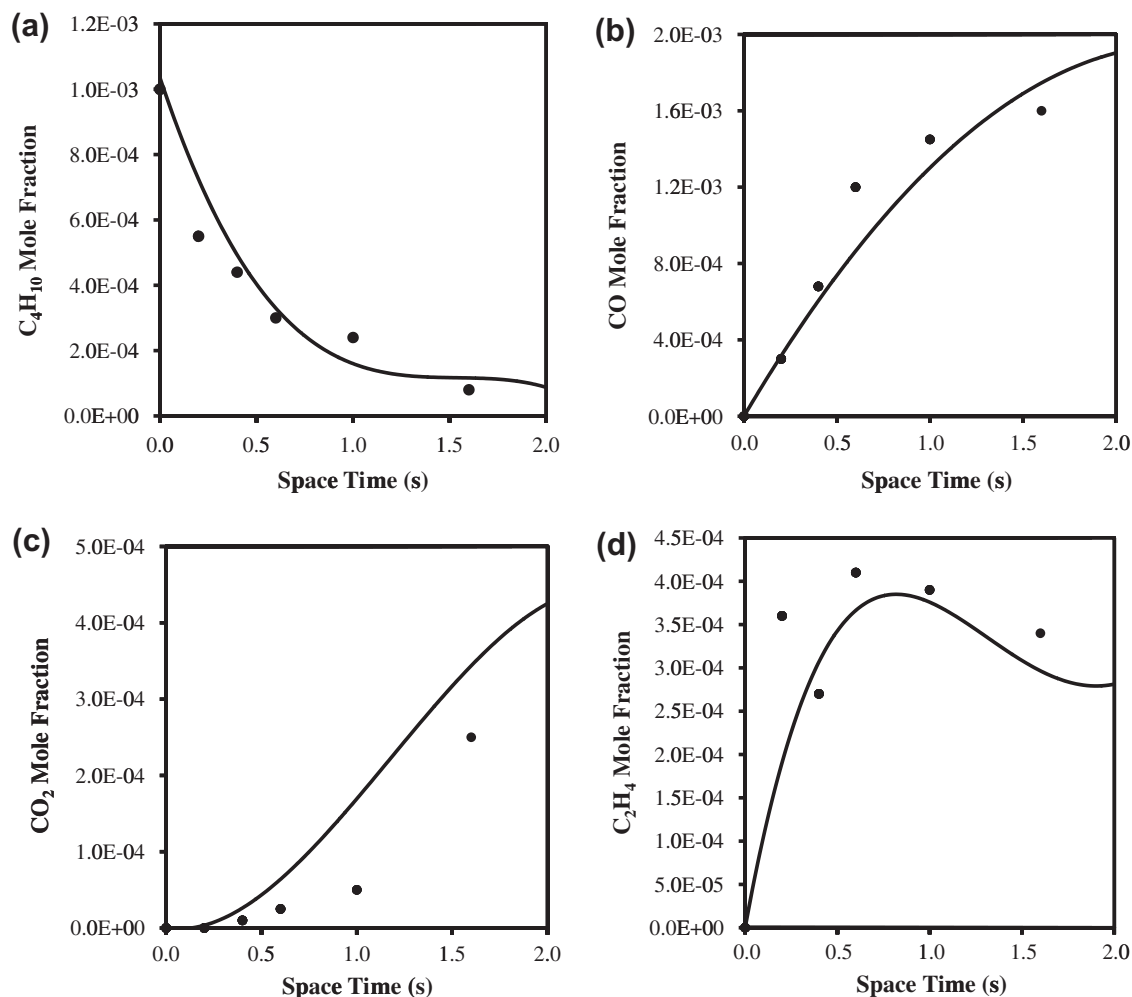


Fig. 1. Validation of the detailed chemical kinetic mechanism by comparison with experimental data [17] for C₄H₁₀ oxidation: Mole fractions of (a) C₄H₁₀, (b) CO, (c) CO₂, and (d) C₂H₄. Lines show modeling results and the symbols correspond to experimental data.

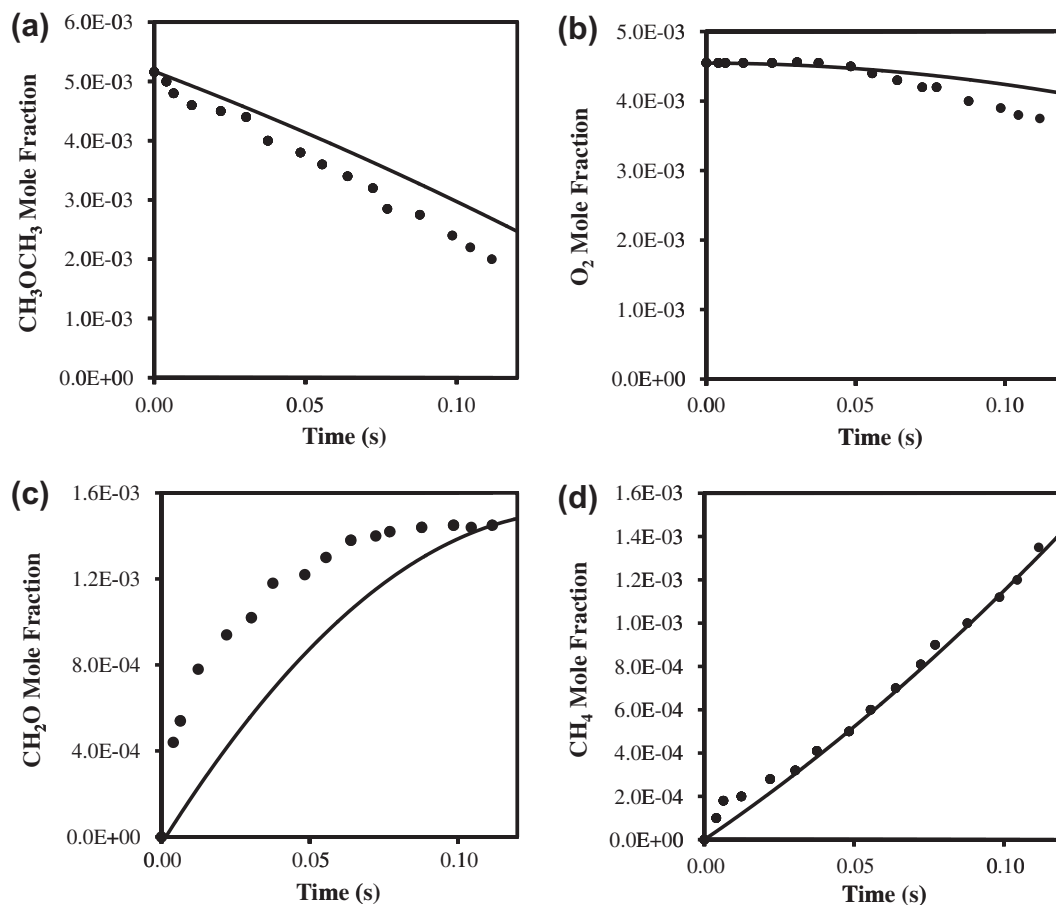


Fig. 2. Validation of the detailed chemical kinetic mechanism by comparison with experimental data [18] for CH_3OCH_3 oxidation: Mole fractions of (a) CH_3OCH_3 , (b) O_2 , (c) CH_2O , and (d) CH_4 . Lines show modeling results and the symbols correspond to experimental data.

Table 1

Inlet mole fractions of the fuels and the oxidizer in $\text{C}_4\text{H}_{10}/\text{CH}_3\text{OCH}_3/\text{O}_2/\text{Ar}$ oxidation system.

Equivalence ratio, ϕ	Dimethyl ether (%)	$X_{\text{C}_4\text{H}_{10}}$	$X_{\text{CH}_3\text{OCH}_3}$	X_{O_2}
2.6	0	0.0057	0.0	0.0143
	20	0.0049	0.0012	0.0138
	50	0.0035	0.0035	0.0129
3.0	0	0.0063	0.0	0.0137
	20	0.0055	0.0014	0.0132
	50	0.0039	0.0039	0.0122

content by mass, leakage and lubricity problems due to its low viscosity, and material compatibility problems with most of the elastomers due to its corrosive nature [9,10]. Therefore, some modifications to engine, fuel supply, and fuel injection systems are required for pure DME application in engines.

Although the major potential utilization of DME as an alternative fuel is for CI engines, there are also many studies in the literature on the application of DME/LPG blends in spark ignition (SI) engines. The performance, emission characteristics, and combustion stability of a 2.7 L SI engine operated with DME/n-butane blend containing 0–30% DME (by mass) were investigated by Lee et al. [11]. Pure n-butane was used as LPG in the study. Stable engine operation was obtained for a wide range of engine loads up to 20% (by mass) DME blended fuel. The engine power output was comparable to that of pure n-butane up to 10% DME concentration. However, for DME concentrations of greater than 10% in the fuel blend, engine power output was decreased and break specific fuel

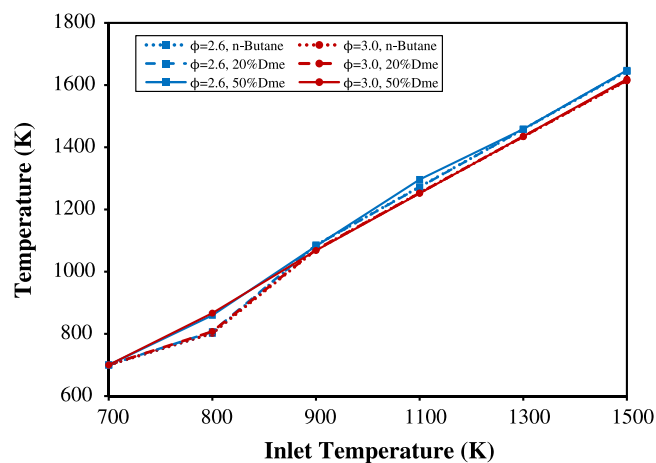


Fig. 3. Final reaction temperatures for different inlet temperatures.

consumption (BSFC) was increased. DME addition to n-butane also increased engine knock. At low engine speed, exhaust THC and NO_x emissions were slightly increased when DME blended fuel was used.

DME blended propane which has a higher octane number than n-butane was also tested in SI engine to reduce the engine knock problem [12]. At a concentration of 20% DME (by mass) in the fuel blend, stable engine operation was obtained for a wide range of engine loads with DME/propane blend rather than DME/n-butane

blend. It has also been reported that engine power output, BSFC, and combustion stability were comparable to those acquired with LPG fuel when propane containing blend was used. The differences in emission levels of CO, THC, and NO_x were not significant for DME/propane and DME/n-butane blends.

Effects of DME addition to gasoline [13], methanol [14], and ethanol [15] on the performance of a modified 1.6 L, four-cylinder SI engine were also investigated experimentally in the literature.

Aromatic species, PAHs, and soot were found to be reduced with the addition of DME to methane, ethane, propane [16,17], and LPG [4]. However, for ethylene, DME addition was observed to increase the formation of PAHs and soot [17,18]. Formaldehyde emissions were reported to increase with DME addition for LPG [4].

To our knowledge, there are no comprehensive studies in the literature investigating the effects of DME addition to n-butane. In this study, the aim was to analyze the formations of major, minor, and trace species in an atmospheric-pressure, adiabatic, tubular reactor for n-butane/DME/oxygen/argon system at two different DME concentrations and two different fuel-rich equivalence ratios using detailed chemical kinetic modeling technique. Equivalence ratio, ϕ , is used to indicate quantitatively whether a fuel-oxidizer mixture is fuel-rich ($\phi > 1$), fuel-lean ($\phi < 1$), or stoichiometric ($\phi = 1$). The amount of the oxidation products formed, especially of the aromatic species and PAHs, are known to be related to the fuel-oxidizer equivalence ratio. Formations of aromatic species and PAHs are observed at fuel-rich conditions, and are known to increase with increasing equivalence ratio. Therefore, for the oxidation of n-butane and DME mixture, two different equivalence ratios at fuel-rich conditions ($\phi = 2.6$ and 3.0) were selected and the

effects of equivalence ratio on the formations of oxidation products were investigated. The reactor inlet temperature was varied from 700 °K to 1500 °K.

2. Method

The detailed chemical kinetic mechanism used in this study was developed by the combination of the oxidation mechanisms of n-butane [19] and DME [20]. This detailed mechanism consisted of 903 elementary reactions of 201 chemical species [21].

The accuracy of the detailed mechanism developed was validated by comparison with the experimental data available in the literature for both n-butane [22] and DME [23] oxidations. The experimental findings in the literature were reproduced by kinetic modeling at the same process conditions, using the detailed chemical kinetic mechanism developed.

Chakir et al. [22] studied n-butane oxidation in a jet-stirred reactor at 937 °K and 10 atm. The kinetic mechanism developed was used to reproduce their results at the same conditions. The model predictions and experimental data are given in Fig. 1 for C₄H₁₀, CO, CO₂ and ethylene (C₂H₄). The detailed chemical kinetic mechanism developed could successfully reproduce the mole fractions of C₄H₁₀, CO, and C₂H₄, while it slightly over predicted the mole fraction of CO₂.

Fischer et al. [23] studied DME oxidation experimentally and theoretically in a flow reactor at 1086 °K and 1 atm, and for an equivalence ratio of 3.4. Their experimental results were reproduced using the kinetic mechanism developed. The results of the

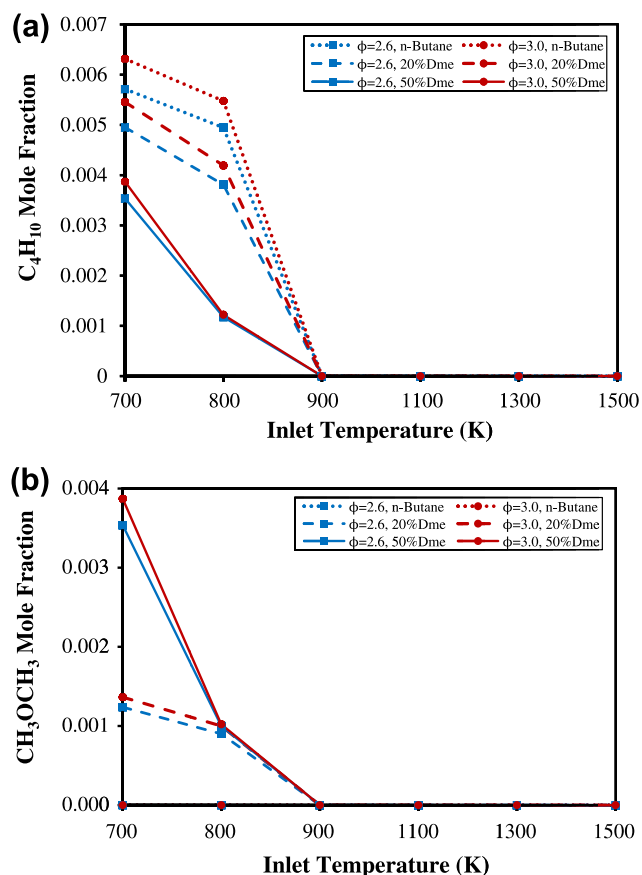


Fig. 4. Mole fractions of (a) n-butane and (b) dimethyl ether at the reactor outlet for different inlet temperatures.

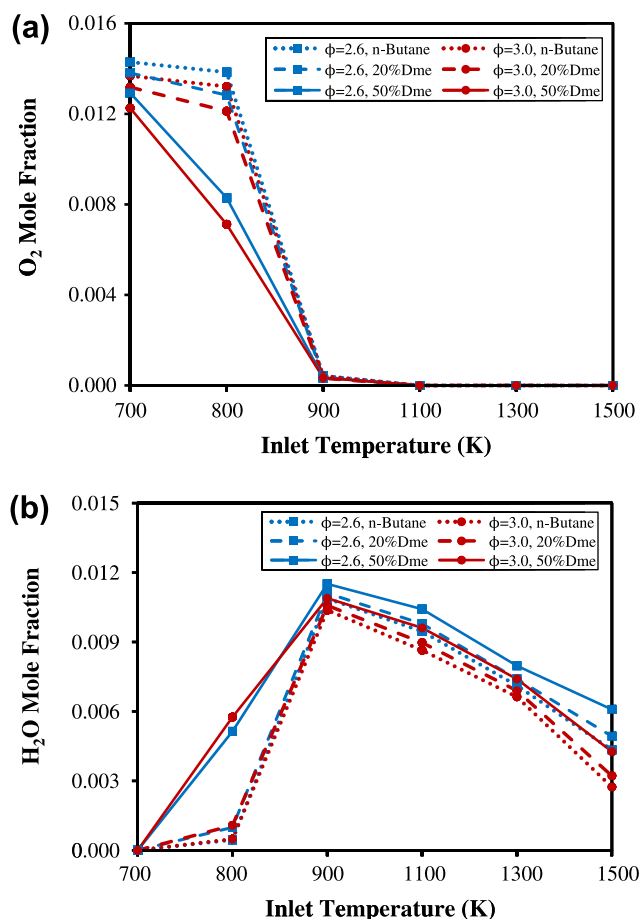


Fig. 5. Mole fractions of (a) O₂ and (b) H₂O at the reactor outlet for different inlet temperatures.

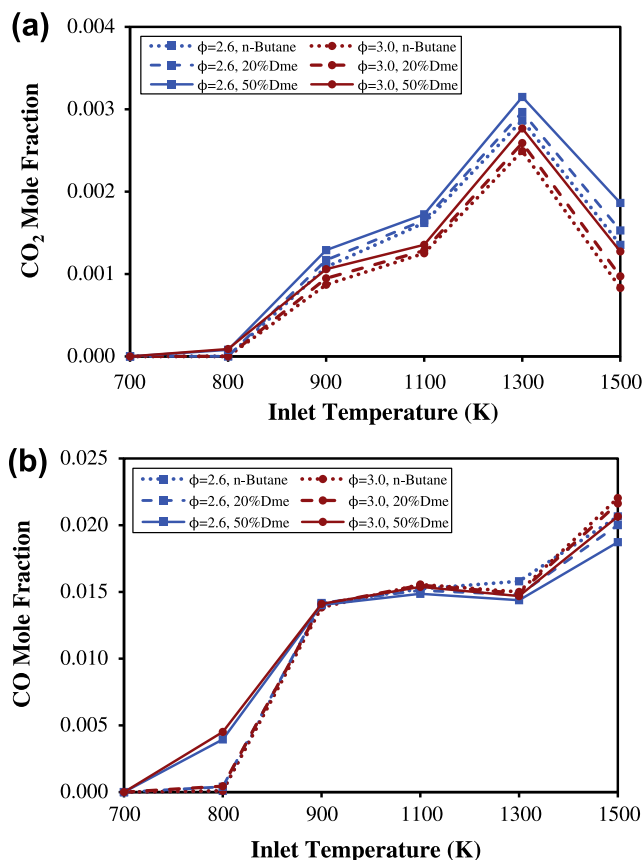


Fig. 6. Mole fractions of (a) CO₂ and (b) CO at the reactor outlet for different inlet temperatures.

comparison between the experimental data and modeling predictions are given in Fig. 2 for CH₃OCH₃, O₂, formaldehyde (CH₂O), and methane (CH₄). The mole fractions of CH₃OCH₃, O₂, and CH₄ were well predicted by the mechanism, while mole fraction of CH₂O was slightly under predicted. Based on these findings, it can be said that the detailed chemical kinetic mechanism developed could successfully predict the mole fractions of various species for the oxidations of n-butane and DME.

Modeling of the n-butane/DME/oxygen/argon system was performed with CHEMKIN-PRO® [24] software, and a tubular reactor with 10 m length and 0.05 m diameter was used for the oxidation process. Flow through the reactor was carried out in laminar flow conditions with a velocity of 0.5 m/s. Plug flow was assumed within the reactor and this assumption was validated according to the dispersion model [25]. The dispersion coefficients calculated for all conditions studied were smaller than 0.01, indicating the validity of the plug-flow assumption. The reactor was operated adiabatically at constant atmospheric-pressure. Six different inlet temperatures ($T_0 = 700, 800, 900, 1100, 1300, \text{ and } 1500 \text{ K}$) were studied, and the concentration profiles of major, minor, and trace species were obtained.

Two different ratios of DME in the inlet fuel mixture (20% and 50%) were studied and the results were compared with those obtained for the oxidation of pure n-butane, in terms of the formations of the oxidation products. The inlet mole fractions of the reactants calculated according to two equivalence ratio values ($\phi = 2.6$ and 3.0), and for different mole fractions of DME in the fuel mixture, are given in Table 1. Argon was used as a diluent gas in the reactor feed mixture, and its mole fraction was kept at 0.98 for all conditions.

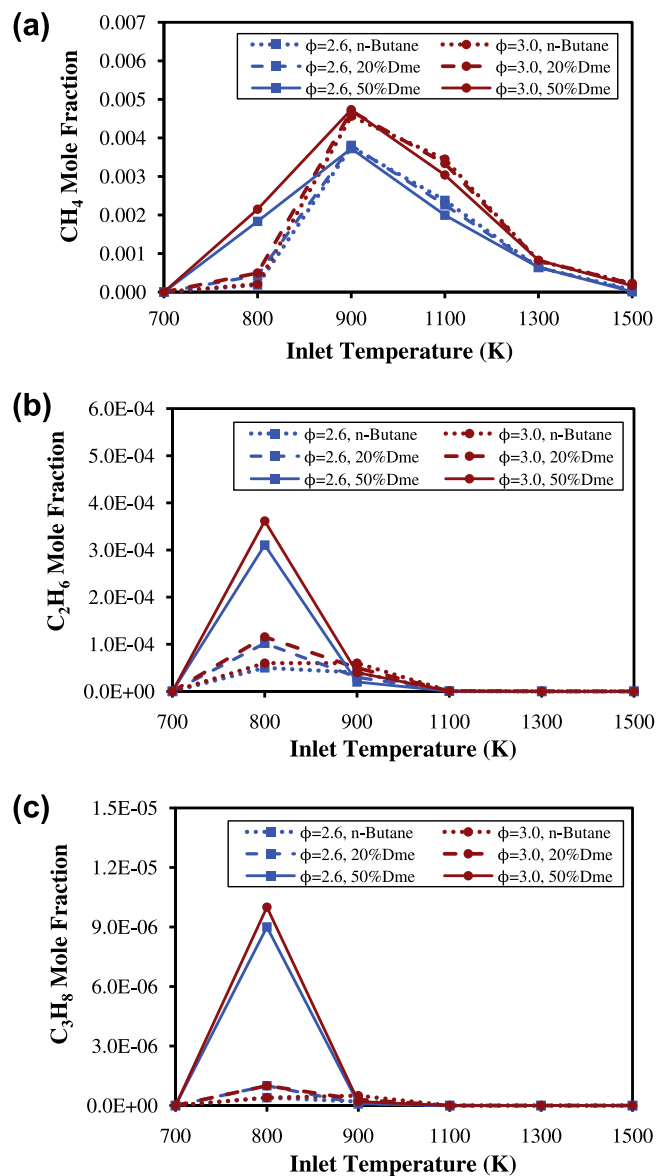


Fig. 7. Mole fractions of (a) methane, (b) ethane, and (c) propane at the reactor outlet for different inlet temperatures.

3. Results and discussion

Mole fractions of various oxidation products at the reactor outlet were obtained for different inlet temperatures, and compared for three different mole fractions of DME (0% (pure n-butane), 20%, and 50%) in the fuel mixture and for two different equivalence ratios (2.6 and 3.0). Final reaction temperatures at the reactor outlet are given in Fig. 3. Final reaction temperatures increased almost linearly with increasing inlet temperatures. The effects of DME mole fraction and equivalence ratio did not seem to have a significant effect on the final reaction temperature, since the temperature rise during reaction was kept at very low levels with Ar dilution.

Fig. 4a and b shows the final mole fractions of n-butane and DME, respectively. It can be observed that the fuels were not totally consumed at the reactor outlet for the inlet temperatures lower than 900 K, where the overall rate of reaction was considerably slow. For the higher equivalence ratio value, the inlet mole fractions of the fuels were higher, and therefore, the outlet mole

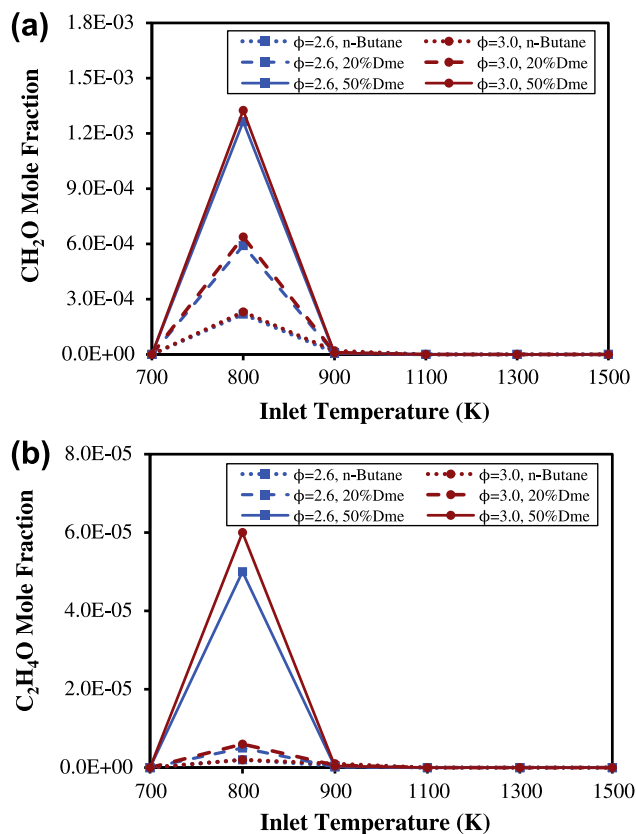


Fig. 8. Mole fractions of (a) formaldehyde and (b) acetaldehyde at the reactor outlet for different inlet temperatures.

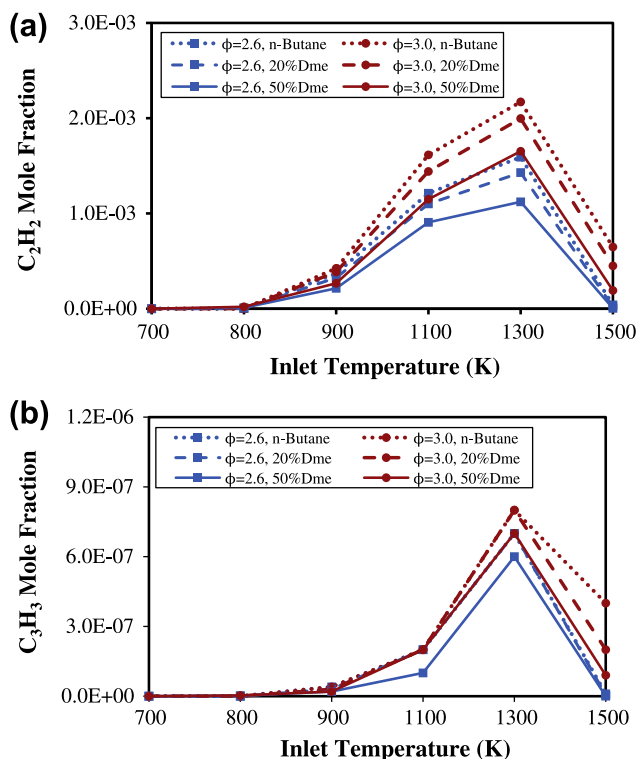


Fig. 9. Mole fractions of (a) acetylene and (b) propargyl at the reactor outlet for different inlet temperatures.

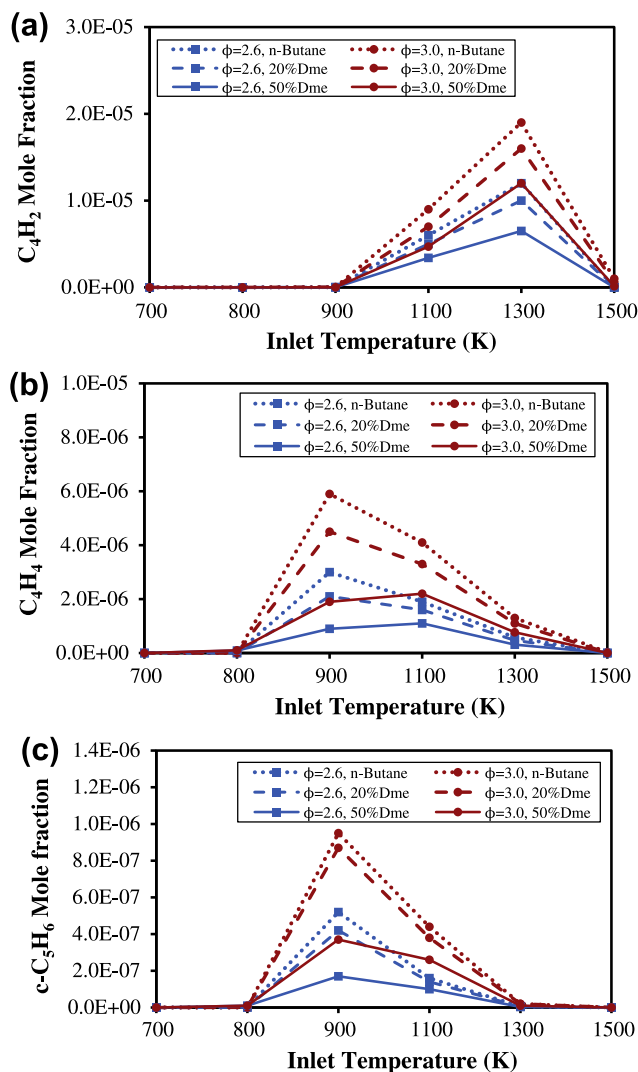


Fig. 10. Mole fractions of (a) diacetylene, (b) vinylacetylene, and (c) cyclopentadiene at the reactor outlet for different inlet temperatures.

fractions were also higher for inlet temperatures lower than 900 °K. For the inlet temperatures of 900 °K and higher, n-butane and DME were totally consumed at the reactor outlet.

Fig. 5a shows the final mole fractions of the oxidizer, O_2 , at the reactor outlet. For the inlet temperatures lower than 900 °K, O_2 was not totally consumed due to the slow reaction rate, similar to the fuels. For the higher equivalence ratio value, the inlet mole fractions of O_2 were lower, and the outlet mole fractions were also lower, for the inlet temperatures lower than 900 °K. For inlet temperatures of 900 °K and higher, O_2 was totally consumed at the reactor outlet.

H_2O is one of the major oxidation products and its mole fractions at the reactor outlet are given in Fig. 5b. The effect of equivalence ratio was apparent for the inlet temperatures of 900 °K and higher. Increasing equivalence ratio decreased the mole fractions of H_2O . Increasing DME mole fraction increased the mole fractions of H_2O at the reactor outlet. Since DME is an oxygenated compound, the increase in the mole fractions of species containing oxygen was expected. The mole fractions of H_2 , and H and OH radicals were also observed to increase with the addition of DME, according to our kinetic mechanism. Maximum mole fraction of H_2O at the reactor outlet was observed for the inlet temperatures of about 900 °K.

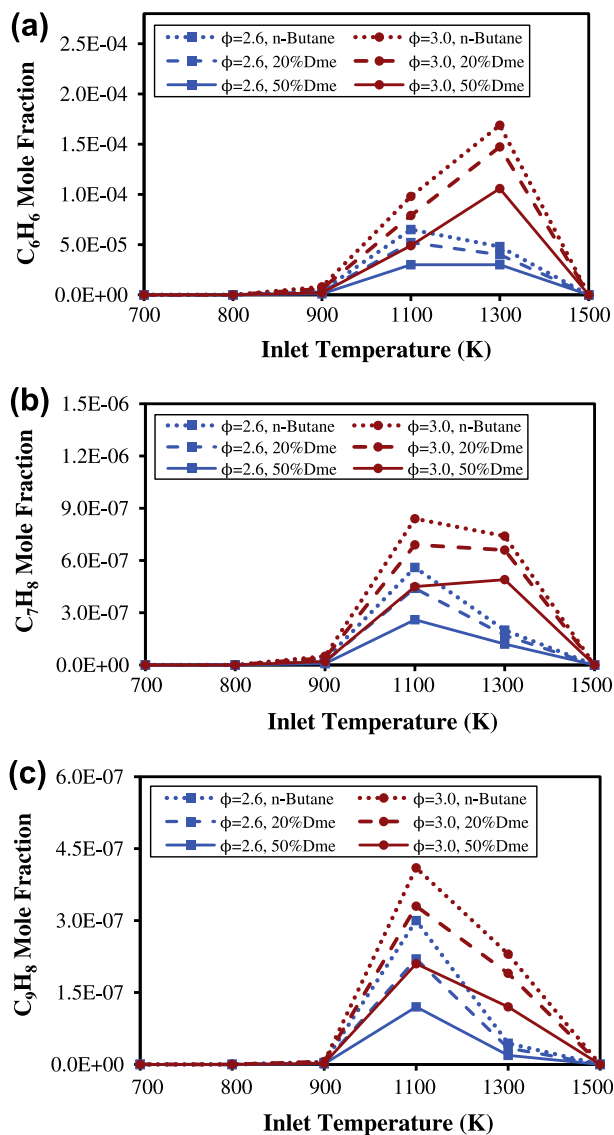


Fig. 11. Mole fractions of (a) benzene, (b) toluene, and (c) indene at the reactor outlet for different inlet temperatures.

Two other major oxidation products are CO_2 and CO , and their mole fractions at different inlet temperatures are shown in Fig. 6a and b, respectively. Increase in the mole fraction of DME increased mole fractions of CO_2 while it decreased mole fractions of CO . The increase in CO_2 and decrease in CO suggested a shift from partial oxidation to complete oxidation. Previously, Frye et al. [5] suggested that DME produced lower CO emissions than propane and butane; and Lee et al. [12] suggested that DME addition to n-butane and LPG decreased the emissions of CO , in conformity with the results obtained in this study. Effect of DME mole fraction on the mole fractions of CO_2 and CO seemed to become more dominant at higher temperatures. Oxygenated structure of DME was considered to increase the mole fractions of CO_2 and H_2O as a result of the reaction $\text{HCOH} + \text{O}_2 = \text{CO}_2 + \text{H}_2\text{O}$. As the mole fraction of CO_2 increased, the mole fractions of CO and CH_2O were considered to be also increasing by the reaction $\text{CH}_2 + \text{CO}_2 = \text{CH}_2\text{O} + \text{CO}$. Then, the mole fraction of CO might have decreased by the reaction $\text{CO} + \text{OH} = \text{CO}_2 + \text{H}$, producing CO_2 , due to the increase in OH radicals. Decrease in the mole fraction of CO was important since CO is an important environmental emission. CO emissions generally increased as the inlet temperature was increased. The effect of equivalence ratio also became more dominant as the inlet temperature

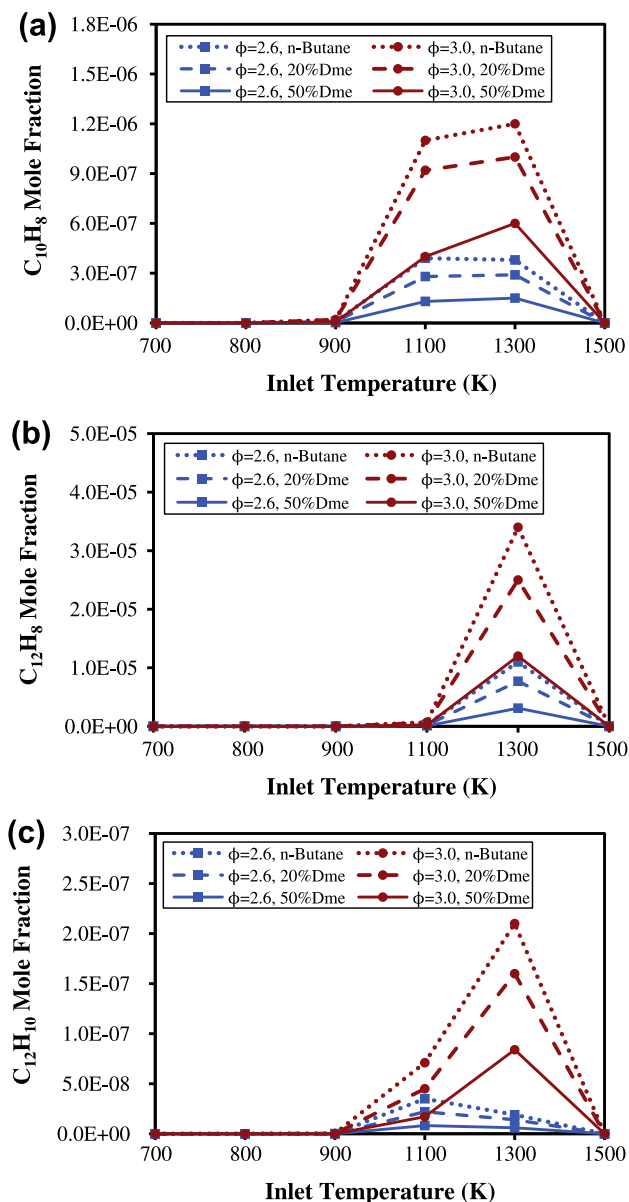


Fig. 12. Mole fractions of (a) naphthalene, (b) acenaphthylene, and (c) biphenyl at the reactor outlet for different inlet temperatures.

was increased. Increasing equivalence ratio increased the mole fraction of CO and decreased the mole fraction of CO_2 .

Methane (CH_4), ethane (C_2H_6), and propane (C_3H_8) are minor oxidation products which are alkanes with smaller carbon numbers than butane, and they indicate C_1 , C_2 , and C_3 oxidation chemistries, respectively. Methane is also important since it is associated with climate change and global warming [26]. Mole fractions of methane, ethane, and propane at the reactor outlet are given in Fig. 7a–c, respectively. Mole fraction of methane did not seem to be affected by the mole fraction of DME significantly. However, mole fractions of ethane and propane increased with increasing DME percentage. In our mechanism, ethane and propane were considered to be mainly produced by the reactions $\text{CH}_3 + \text{CH}_3(+\text{M}) = \text{C}_2\text{H}_6(+\text{M})$ and $\text{C}_2\text{H}_5 + \text{CH}_3(+\text{M}) = \text{C}_3\text{H}_8(+\text{M})$, respectively. The increase in the methyl (CH_3) radicals due to decomposition of DME (CH_3OCH_3) was considered to increase the interaction between these methyl radicals rather than interactions with other radicals, resulting in increases in the formations of ethane and propane, instead of methane. Increasing equivalence ratio

resulted in slight increases in mole fractions of methane, ethane, and propane. Maximum mole fractions of ethane and propane at the reactor outlet were observed around 800 °K, and the maximum mole fraction of methane was observed around 900 °K.

Although DME is known to reduce the formations of several toxic oxidation products when used as a fuel additive, in previous studies it was shown that DME addition to butane and butane/propane mixtures increased the formation of another toxic species, formaldehyde [4]. The mole fractions of formaldehyde obtained in this study for different mole fractions of DME and two different equivalence ratios are shown in Fig. 8a. Acetaldehyde (C_2H_4O) is another aldehyde with two carbons and its mole fractions at the reactor outlet are given in Fig. 8b. Both aldehydes were observed to increase as the DME percentage was increased. The oxygenated structure of DME promoted the formations of these oxygenated species. In our mechanism, the increase in the mole fraction of formaldehyde was considered to be resulting from the reactions $CH_3 + OH = CH_2O + H_2$, $CH_3O(+M) = CH_2O + H(+M)$, and $CH_2OH + O_2 = CH_2O + HO_2$, due to the oxidation chemistry of DME. The increase in the mole fraction of acetaldehyde might be related to the reactions $CH_3 + HCO = C_2H_4O$ and $pC_3H_5 + O_2 = C_2H_4O + HCO$, due to the oxygenated structure of DME and the increase in the CH_3 radical concentration. The effect of equivalence ratio did not seem to be significant under the conditions studied. The maximum mole fractions of these species were observed at around inlet temperatures of 800 °K.

PAHs constitute an important class of toxic species from the combustion of hydrocarbon fuels. They are high molecular weight aromatic species composed of two or more aromatic benzene (C_6H_6) rings and some members of PAHs are known to be mutagenic or carcinogenic. They are also precursors of soot formation. Formations of aromatic species and PAHs occur at fuel-rich conditions. Some minor oxidation products are known to be the precursors of formations of aromatic species and PAHs [27]. In this study, among these precursors, two-carbon-number acetylene (C_2H_2), three-carbon-number propargyl (C_3H_3), four-carbon-number diacetylene (C_4H_2), and vinylacetylene (C_4H_4), and five-carbon-number cyclopentadiene ($c-C_5H_6$) were investigated.

Fig. 9a shows the mole fractions of acetylene at the reactor outlet. Increasing DME mole fraction decreased mole fractions of acetylene. Acetylene is known to react with C_4 species to form benzene and other aromatic rings, and it also reacts with aromatic species to form larger PAHs [28,29]. According to our mechanism, as DME was added, the reactions of C_2H_2 with O and OH radicals and O_2 , producing smaller C_2 and C_1 species, were considered to lower the mole fraction of C_2H_2 . Fig. 9b shows the mole fractions of propargyl at the reactor outlet. Propargyl is known to react with other C_3 species to form aromatic rings [30,31], and increasing DME mole fraction slightly decreased mole fractions of propargyl.

Fig. 10a and b shows the mole fractions of diacetylene and vinylacetylene, respectively. These two acetylenic molecules are also suggested as precursors of PAHs in the literature [28,29]. Increasing DME percentage decreased mole fractions of these two species. Diacetylene was considered to be produced in lower amounts from acetylene by the reaction $C_2H + C_2H_2 = C_4H_2 + H$, according to the mechanism developed, since the mole fraction of acetylene was also decreased. Similarly, vinylacetylene production by the reaction $C_2H_3 + C_2H_2 = C_4H_4 + H$ was decreased with the decrease in the mole fraction of acetylene. Fig. 10c shows the mole fractions of cyclopentadiene at the reactor outlet. Increasing DME mole fraction also decreased mole fraction of cyclopentadiene. Similar to diacetylene and vinylacetylene, cyclopentadiene was also formed by the reaction $aC_3H_5 + C_2H_2 = c-C_5H_6 + H$ from acetylene in lower amounts, according to our mechanism, with the addition of DME.

Increasing equivalence ratio increased the mole fractions of the entire precursor species investigated. Maximum mole fractions of

acetylene, propargyl, and diacetylene at the reactor outlet occurred at around inlet temperatures of 1300 °K, while maximum mole fractions of vinylacetylene and cyclopentadiene occurred at around inlet temperatures of 900 °K.

Among the aromatic species and PAHs that are formed as a result of oxidation processes, one-ring benzene (Fig. 11a), toluene (C_7H_8) (Fig. 11b), and indene (C_9H_8) (Fig. 11c), and two-ring naphthalene ($C_{10}H_8$) (Fig. 12a), acenaphthylene ($C_{12}H_8$) (Fig. 12b), and biphenyl ($C_{12}H_{10}$) (Fig. 12c) were investigated. Increasing DME mole fraction decreased the mole fractions of all of these aromatic species. This was an expected result, since DME addition also decreased the mole fractions of the precursor species investigated. Larger PAH molecules that were not investigated in this study are also expected to decrease with the addition of DME, since they are formed by acetylene addition to smaller aromatic rings or by recombination of these smaller rings [27]. Increasing equivalence ratio increased mole fractions of all of these aromatic species. Maximum mole fractions of these aromatic species at the reactor outlet were observed at around inlet temperatures of 1100 and 1300 °K.

4. Conclusion

The effects of DME on the formations of various products from n-butane oxidation were investigated by detailed chemical kinetic modeling. Two different DME concentrations and two fuel-rich equivalence ratios were studied for six different values of reactor inlet temperatures. Oxidation process was carried out in an adiabatic tubular reactor under constant atmospheric-pressure condition. The results were compared with those obtained for the oxidation of pure n-butane.

The addition of DME decreased the formations of toxic species such as CO, aromatic species, and PAHs, released from the oxidation of n-butane. However, the mole fractions of formaldehyde and acetaldehyde were increased.

Mole fractions of CO, methane, aromatic species, and PAHs were increased with an increase in the equivalence ratio. The effects of equivalence ratio on the mole fractions of formaldehyde and acetaldehyde were not significant under the conditions studied.

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