A chemical kinetic study of low alcohol/iso-octane blends in both premixed and partially premixed combustion

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Abstract
The use of alcoholic fuels in both compression ignition and spark ignition engines has received much attention in recent years. Using these fuels, either in pure form or in a blended form with gasoline, not only reduces engine emissions but also improves engine performance. Therefore, a careful examination of the chemical kinetics of combustion of alcoholic fuels is of great importance. Since the run time of combustion chemistry calculations is proportional to the square of the total number of species in the chemical kinetic mechanism, the use of a detailed chemical kinetic mechanism for engine design and optimization is not practical. In this paper, first, the performance of a reduced mechanism has been investigated in terms of predicting ignition delay time and laminar flame speed. Then, the mechanism is utilized to study and compare three different blends of alcohol fuels (namely methanol and ethanol) and iso-octane with identical stoichiometric air to fuel ratio, volumetric energy content, octane numbers and latent heat. Combustion properties for both premixed and non-premixed diffusion flames, and homogeneous reactor configurations are studied. The results indicate that ignition delay and laminar flame speed are more defined by the iso-octane and methanol content rather than ethanol. Generally, blends with lower iso-octane and higher methanol give a longer ignition delay time and a higher laminar flame speed. The main source of pollutant formation for one of the blends are also discussed.

Introduction

Internal combustion (IC) engines are commonly used as the main propulsion system for air, ground and rail vehicles. The use of fossil fuels for these engines often raises concerns about the environment and pollutants from combustion. Therefore, the use of alternative fuels, such as methanol and ethanol, has received much attention in recent years due to their unique properties in improving the performance and reducing emissions of IC engines. Methanol and ethanol have high enthalpy of vaporization and low stoichiometric air-fuel ratio, resulting in a cooling effect, which can reduce NOx emissions, and increase knock resistance and volumetric efficiency [1, 2]. In addition, their low adiabatic flame temperature, higher flame speed, and higher octane number allow to design a spark ignition engine with higher compression ratio, higher intake airflow boosting, and higher rate of cooled EGR which are beneficial to reach higher efficiency, and maximum achievable load [3]. Because they can produced from different sources, they may decrease the dependency on oil import which leads to a higher energy security [4]. Ethanol and Methanol can be made from biological sources that allow countries to produce fuel within their borders by growing plants, which will lead to a reduction in greenhouse gases [5]. Currently methanol is mostly produced from fossil fuels [6]. Both however can be synthesized from hydrogen and carbon dioxide [7], which within the context of CCS and e especially BECCS, offer an excellent long term perspective.

Table 1 summarizes the physicochemical properties of iso-octane, ethanol and methanol. By considering the characteristics of the fuels, methanol and ethanol can be

excellent alternative fuels in spark ignition engines both from a production and an end-use point of view. They can be used in a pure form, or binary and ternary mixture with gasoline fuel since they are soluble in gasoline. They also have the capability to be utilized in the strategy, so-called 'octane-on-demand', i.e. gasoline is used for most operating conditions, and methanol or ethanol are used when there is a high probability of knock occurrence [8, 9]. Being in liquid form, they are consistent with existing infrastructure and can be easily stored in the car. At present, the use of ethanol and methanol in gasoline with low level blend ratio is fully commercialized. Modern gasoline contains 5% in volume. E5 and E10 are now being introduced in Europe and the United States. In addition, In Europe, 3% methanol is allowed to be mixed in gasoline until the overall oxygen concentration do not exceeds 3.7% by mass [10]. Turner et al. [11] discovered reduced CO_2 and NOx emissions by binary mixture of ethanol and methanol (60–70 vol% methanol and ethanol) with gasoline, compared to the pure gasoline. Sileghem et al. [12] found out lowered CO and NOx emissions using the binary blend compared to the neat gasoline. Elfasakhany [13] used lower blend ratio (3–10 vol% ethanol and methanol) with enhanced performance and emissions characteristics. Nazzal [14] observed similar results with blends at rate of 6, 6 and 88 vol% for ethanol, methanol and gasoline, respectively. Vancoillie et al. [15] discovered reduced NOx and CO_2 emissions and improved thermal efficiency with methanol/gasoline blend compared with that of a pure-gasoline. Recently, Tian et al. [16] showed that adding alcohol fuels to gasoline can increase the brake torque and heat release rate of the engine. Moreover, the ability of methanol to increase torque and heat release rate is higher than that of ethanol. Compared to ethanol, methanol can better

increase the brake thermal efficiency of the engine, but it also increases brake specific fuel consumption even more. In terms of emissions, the addition of alcohol fuels to gasoline can reduce CO and CO_2 emissions, but HC emissions are increased.

Table 1. Physicochemical properties of studied fuels [1, 17].

Properties	Iso-octane (C_8H_{18})	Ethanol (C_2H_5OH)	Methanol (CH_3OH)
Molecular weight [kg/kmol]	114	46	32
Density at 298 K and 1 atm (kg/m³)	692	790	790
Oxygen content (% weight)	21.62	34.8	50
Heat of vaporization [kJ/kg]	270	838	1100
Theoretical air-fuel ratio	15.13	9.0	6.4
Lower heating value (MJ/kg)	44.65	26.77	19.92
Flammability limit (vol.%)	1.1–6.0	4.3–19	6.0–36.5
Auto-ignition temperature (°C)	447	420	470
Latent heating (MJ/kg)	0.283	0.904	1.088
Volumetric energy content [MJ/m³]	30656	21291	15871
Adiabatic flame temperature (K) at $\Phi=1$	2276	2193	2143

Methanol and ethanol can also be mixed with diesel in compression ignition engines so that the blended fuels can enhance the overall engine's performance characteristics. For a compression ignition engine, the mixing of alcohol additives with diesel fuel supplies the oxygen required to form CO_2 instead of carbon-rich particles, thus may considerably reduce PM emissions [18]. Zhu et al. [19] found higher maximum pressure, heat release rate, thermal efficiency and ignition delay period and lowered emissions of CO, HC, NOx and PM with ethanol/diesel blend compared with pure diesel case. Ajav et al. [20] realized a decrease in CO and NOx emission with ethanol/diesel blend. Li et al. [21] noticed higher brake specific fuel consumption and brake thermal efficiency and lower CO and NOx emission. Sayin [22] experimented methanol/diesel blend and represented lower CO, HC and smoke emissions because of oxygen content of methanol and more complete combustion compared with pure diesel case. Jamrozik et al. [23] experimentally studied a dual fuel system, in which co-combustion for diesel and methanol and ethanol with energy contents of 20%, 30%, 40% and 50% was carried out. It was shown that the presence and increase in the share of methanol and ethanol used for co-combustion with diesel fuel causes an increase in ignition delay and increases the heat release rate and maximum combustion

pressure values. A larger ignition delay is observed for co-combustion with methanol.

Although methanol and ethanol addition have shown improved performance and lower emissions, methanol and ethanol have limited solubility in diesel; hence the blend ratio in diesel are limited to small percentages [24]. Therefore, they are more common to be used as pre-mixed fuel in advanced compression ignition strategies such as dual-fuel reactivity-controlled compression ignition (RCCI) engines [25-28]. Use of ethanol as the premixed fuel in dual fuel operation was investigated experimentally by Han et al [29]. The results showed increased efficiency at medium loads and lower soot emissions compared to conventional diesel engines. The higher flame speed of premixed fuel can result in lower HC-CO emissions in RCCI engines [30, 31]. As a result, they can address high HC-CO emissions problems in RCCI engines.

Due to the unique properties of these fuels, the chemical kinetic analysis of these fuels either in pure form or in blended form with gasoline in engine relevant conditions is of particular importance and a deep understanding of their properties is very helpful for use in engine designs. The chemical kinetic mechanism used for heavy hydrocarbon fuels usually has a large number of chemical species and reactions. The use of such mechanisms in the modeling of internal combustion engines and the study of the chemical kinetics of fuel is practically impossible due to their high computational time, and therefore it is preferable to use so-called reduced mechanisms, which have a much smaller number of species and reactions. In this paper, the performance of a chemical kinetic mechanism is examined, which has a lower number of species and reactions, while providing good accuracy for predicting the chemical kinetic properties of methanol, ethanol and gasoline. After proving that the mechanism used has good accuracy in predicting fuel properties, it is utilized to investigate combustion properties of three different blends with identical stoichiometric air to fuel ratio, volumetric energy content, octane numbers and latent heat in both a premixed and a non-premixed configuration. Finally, homogeneous reactor simulation will be performed to study pollutant formation.

Chemical Kinetic Mechanism Validation

The chemical kinetic mechanism used in this paper is a reduced mechanism consisting of 80 species and 349 reactions [32]. This mechanism is one of the main kinetic models used in the literature to simulate alcohol and iso-octane ignition delay times (IDT) and laminar flame speed (LFS). In order to use this mechanism, the accuracy of this mechanism, in predicting the properties that are to be examined, must first be evaluated. In order to assess the accuracy of the mechanism, the predicted results of the properties by the mechanism must be compared with the existing experimental results. A set of experimental data was extracted from the literature for validation and are summarized in Table 2.

One of the most important parameters for validating the chemical kinetic mechanism is the ignition delay time. Ignition delay time of the mixture has a direct effect on the amount of energy released in the engine cylinder and the occurrence of knock and engine emissions [33]. Fuels with longer ignition delay are more resistant to autoignition, therefore in both SI engine and Dual Fuel engine, higher operating loads can be achieved with stable operation. Laminar flame speed (LFS) of the mixture is another key parameter which has a direct effect on the emissions levels, flammability limits, reactivity, and combustion efficiency of engines [33, 34]. Fuels with higher flame speed make more room for engine designer to obtain higher efficiency and lower carbon emissions.

In this paper, Cantera and CHEM1D are used to calculate the thermodynamic and chemical kinetics properties of ternary mixtures of ethanol, methanol and gasoline. Cantera and CHEM1D are open source software for analyzing 0D and 1D reactive systems [35, 36]. In 0D system, the ignition delay time is calculated by the maximum point of OH concentration curve, and in 1D counter flow configuration, ignition delay is defined by the time when the position of the OH concentration equal to 2% of the maximum found in the simulation. This location defines the IDT according to the commonly used definition in the engine combustion network (https://ecn.sandia.gov/). Laminar flame speeds are calculated by freely-propagating, adiabatic, 1-D flame using the mixture-average formulation for the transport properties. Soret effects and radiation losses were ignored.
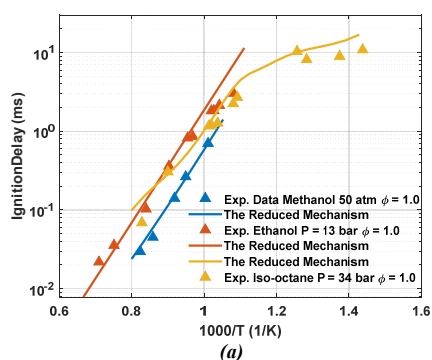
Table 2. Experimental conditions for the ignition delay time and laminar flame speed simulation of Isooctane, ethanol, and methanol reported in the literature.

Fuel	ϕ [-]	T[K]	P[atm]	Reference
Ignition Delay Time				
Methanol	1	990-1210	50	[37]
Ethanol	1	924-1408	12.8	[38]
Iso-octane	1	695-1205	33.5	[39]
N-heptane	1	750-1065	41	[40]
N-heptane	1	735-1065	30	[40]
Laminar Flame Speed				
Methanol	0.7-1.5	343	1	[41]
Ethanol	0.7-1.5	298	1	[42]
Iso-octane	0.7-1.5	300	1	[43]
N-heptane	0.6-1.4	298	1	[44]

Results and discussion
Ignition delay times and laminar flame speeds
The predicted ignition delay time for Methanol, Ethanol, Iso-octane and N-heptane in air as a function of temperature is shown in Fig. 1. Results are compared with the experimental data from the previous published works which have been mentioned in Table 2. A good agreement with experimental results is obtained. The results show that the mechanism reproduces the experimental data well. To ensure that the model used can predict the NTC behavior for n-heptane, two operating conditions are studied. The mechanism captures the NTC behavior in both cases. There is only a very small difference between predicted and measured values.
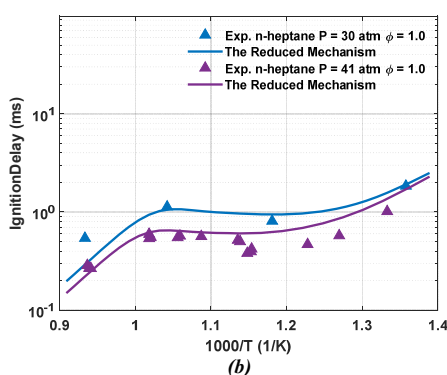

Fig. 1. Comparison of IDT profiles simulated to those measured experimentally for (a) Methanol/air, at P = 50 atm and φ = 1.0; ethanol/air, at P = 13 bar and φ = 1.0; Iso-octane/air, P = 40 bar and φ = 1.0 (b) N-heptane/air, P = 30 atm and φ = 1.0; N-heptane/air, P = 41 atm and φ = 1.0

The predicted laminar flame speed for Methanol, Ethanol, Iso-octane, and N-heptane in air as a function of equivalence ratio is shown in Fig. 2 for athmospheric conditions since experimental results for higher pressures are rare. Perfect agreement between the experimental data reported in Table 1 and the values predicted by the chemical mechanism is seen in the range of equivalence ratios between 0.7 and 1.5. As it can be seen, the mechanism used reproduces the experimental values for mixtures of methanol/air and gasoline/air well, and only overpredicts the laminar flame speed for ethanol/air mixture in very rich conditions. Overall, the current chemical mechanism can estimate previously published results of laminar flame speeds and ignition delays and can be used for further kinetics studies.
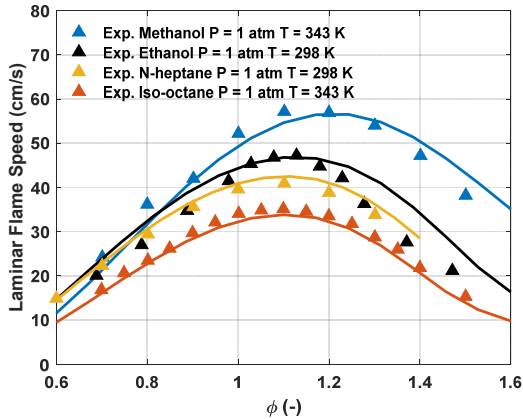
Fig. 2. Comparison of LFS profiles simulated to those measured experimentally for Methanol/air, at P = 1 atm and T = 343 K; Ethanol/air, at P = 1 atm and T = 298 K; Iso-octane/air, P = 1 atm and T = 300 K; N-heptane/air, P = 1 atm and T = 298 K.

The plots in Fig. 3 shows the ignition delay times and laminar flame speeds of iso-octane/ethanol/methanol/air mixtures at $p = 60$ atm, T=900K and equivalence ratio of 0.7 (a representative condition for the premixed charge in a dual fuel compression ignition engine at the start of injection). Usually, a longer ignition delay and the larger flame speed are beneficial in dual-fuel- and also spark-ignition engines, because the longer ignition delay means higher resistance to autoignition which causes the engine to achieve higher operating loads with a more stable performance. Also, higher flame speed will cause the fuel-air mixture to burn faster, which will reduce unburned hydrocarbon and carbon monoxide emissions, not to mention increase efficiency. Each point inside the triangle corresponds to a specific combination of the three fuels. For example, the point in the plot with the three arrows represent the mixture with a volume fraction of CH3OH of 40%, 40% C2H5OH, and 20% IC8H18. It is shown that the addition of small amounts of ethanol and methanol to iso-octane considerably increases the ignition delay time. This is mainly due to single stage auto ignition characteristics of ethanol and methanol, because they do not have cool flame. It is also apparent that by increasing the percentage of the methanol and ethanol in the blend laminar flame speed increases significantly due to the higher laminar flame speeds of ethanol and methanol compared to iso-octane. The results of ignition delay and laminar flame speed for three different ternary blends are presented. The blends are selected such that they have the same stoichiometric air to fuel ratio as conventional E85 (85 v/v% ethanol and 15 v/v% gasoline). Turner et al. [11] have shown that these have also an identical volumetric energy content (based on the masses and densities of the individual components), constant octane numbers and constant latent heat. The naming convention of the blends is such that the first letter indicates the type of fuel and the number following the letter indicates the volume percentage of fuel in the blend. As we can see the ID and LFS results are more dependent on iso-octane and methanol rather than ethanol content. Generally, the blends with a lower iso-octane and a higher methanol content show a higher IDT and LFS.
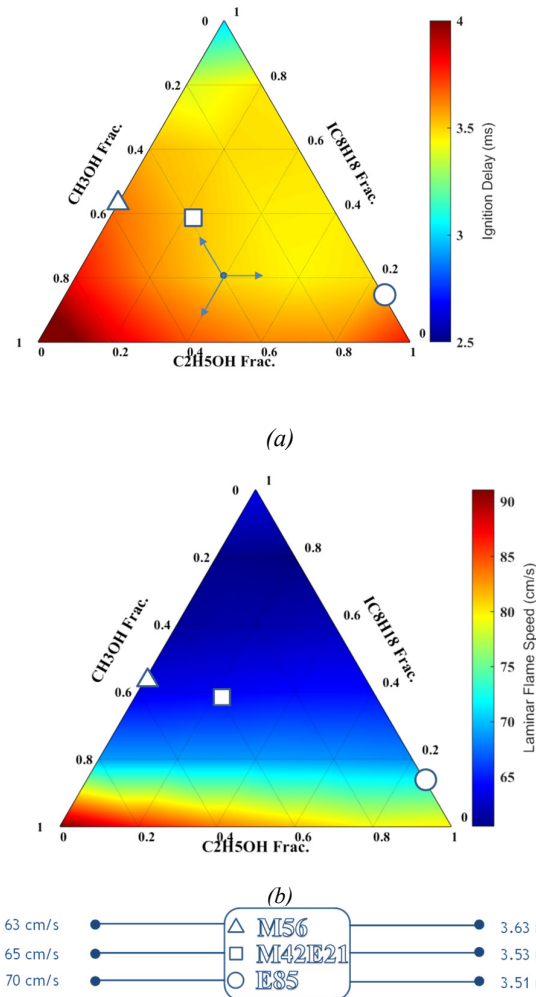

(a)

(b)

63 cm/s	△ M56	3.63 ms
65 cm/s	□ M42E21	3.53 ms
70 cm/s	○ E85	3.51 ms

Fig.3. Ternary contour plot for: a) ignition delay times and (b) laminar flame speeds of iso-octane/ethanol/methanol/air mixtures at $p = 60$ atm, T = 900 K, and Phi = 0.7

Laminar counter flow diffusion flame

The study of this type of flame serves as a basis for many combustion models for diesel engine combustion (e.g. RIF, FGM). For dual-fuel compression ignition (DFCI) engines, both a premixed flame and a diffusion flame will form. An auto-igniting counterflow configuration with premixed and a non-premixed side (Partially premixed counterflow diffusion flame, PPCDF) may serve as a conical configuration for such a DFCI engine. Therefore, a particular classical counterflow set-up is studied to establish the performance of the reaction mechanism in a dual-fuel situation. Certainly, an accurate mechanism should work well in both premixed and non-premixed mode.

The schematic diagram of the counter flow flame is shown in the Fig. 5. On the 'oxidizer'-side now a pre-mixed mixture of air and alcohol/i-octane blend is defined and on the other side pure n-heptane.
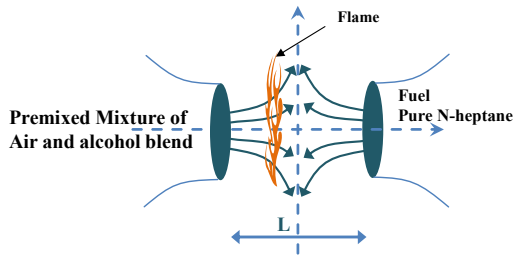
Fig.5. schematic diagram of partially premixed laminar counter flow diffusion flame (PPCDF). Premixed side conditions: P = 60 atm, T = 900 K, Phi = 0.7

M56 and M42E21 were chosen for further study as function of the applied strain rate (a measure for the velocity at the nozzle exits in the counterflow configuration) as they have a more similar alcohol and iso-octane content when we compare them with E85. The temperature profiles at different times are presented in mixture fraction space in Fig. 6. As time advances the temperature raises until it reaches the steady state solution. The black line connects the maximum values of temperature for each time. It can be seen that the trajectory through mixture fraction space is quite similar. However, as function of time there is a clear difference. Fig. 7 shows the maximum temperature for different strain rates as function of time. The small circles in the profiles represents the position of the OH concentration equal to 2% of the maximum found in the simulation. This location defines the IDT according to the commonly used definition in the engine combustion network (https://ecn.sandia.gov/). As it can be seen the case of the M56 blend ignites earlier which shows that even small difference in iso-octane content has influence on ignition properties. As also can be seen in Fig. 8 where IDT is directly plotted against strain rate, a higher i-octane content ignites earlier. Their results were also compared to the case where pure air is present in the oxidizer side.
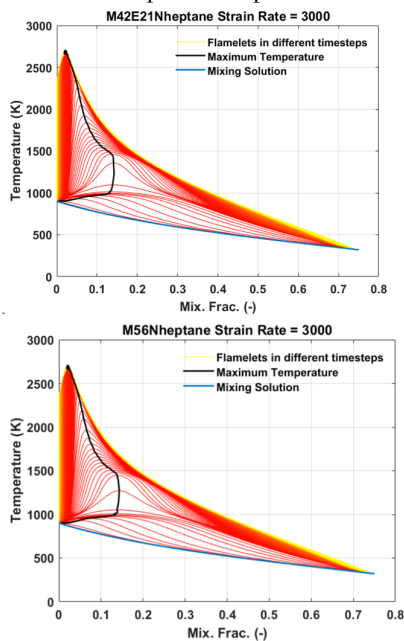

Fig.6 maximum temperature profiles in different times in PPCDF with different fuel blends (top: M42E21, bottom:M56) at premixed side at strain rate of 3000 1/s and P = 60 atm. Premixed side conditions: T = 900 K, Phi = 0.7
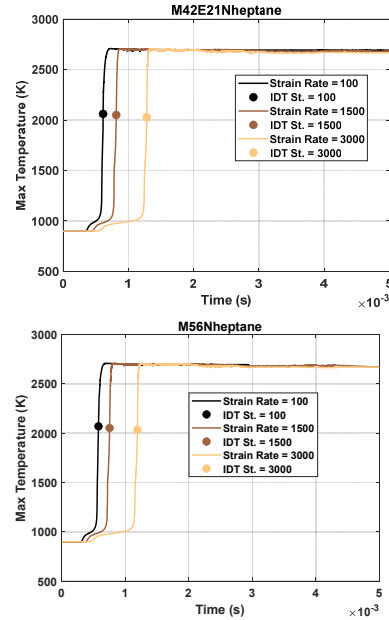

Fig.7 maximum temperature against time in a PPCDF with different blends (top: M42E21, bottom:M56) at the oxidizer side for different strain rate at P = 60 atm. oxidizer side conditions: T = 900 K, Phi = 0.7.
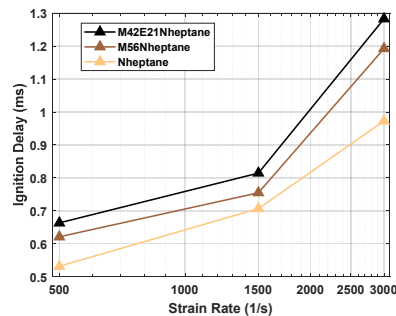

Fig.8 Ignition delay time against strain rate in laminar counter flow diffusion flame for two different blends and pure air in the premixed side. Premixed side conditions for the two blends: P = 60 atm, T = 900 K, Phi = 0.7

Pollutant formation
The mechanism was utilized to do a homogeneous reactor simulation to study emissions formation at constant pressure and temperature at various initial mixture equivalence ratios and temperatures as done by Kitamura for soot and NOx in the so-called phi-T maps [45]. M42E21 was used as a representative of alcohol fuel blend with gasoline. It has been shown that the interpretation of these phi-T maps are very useful to interpret experiments [46]. The results have been depicted in Fig. 9. The main source of CO emissions originates from very rich regions where there is not

sufficient oxygen to convert CO to CO2, and despite diesel combustion, there is no source of CO emission in lean regions [46]. In diesel combustion, high CO emissions at lean conditions are usually observed in temperatures lower than 1400 K where fuel is overmixed and burns slowly (the conditions in low load operation of diesel engines). Here we do not see such high CO region. The main source of CO emissions are in high temperature and equivalence ratio where the temperatures are high enough to oxidize fuel but O2 concentrations are not adequate to make combustion complete (see CO2 map for the region with incomplete combustion). The main source of NOx emission is in the lean and high temperature region where both temperature is high and the oxygen remains to form NOx emission. Also, the rate of NOx formation is sharper at T>1800 K which is consistence with the finding of [47].
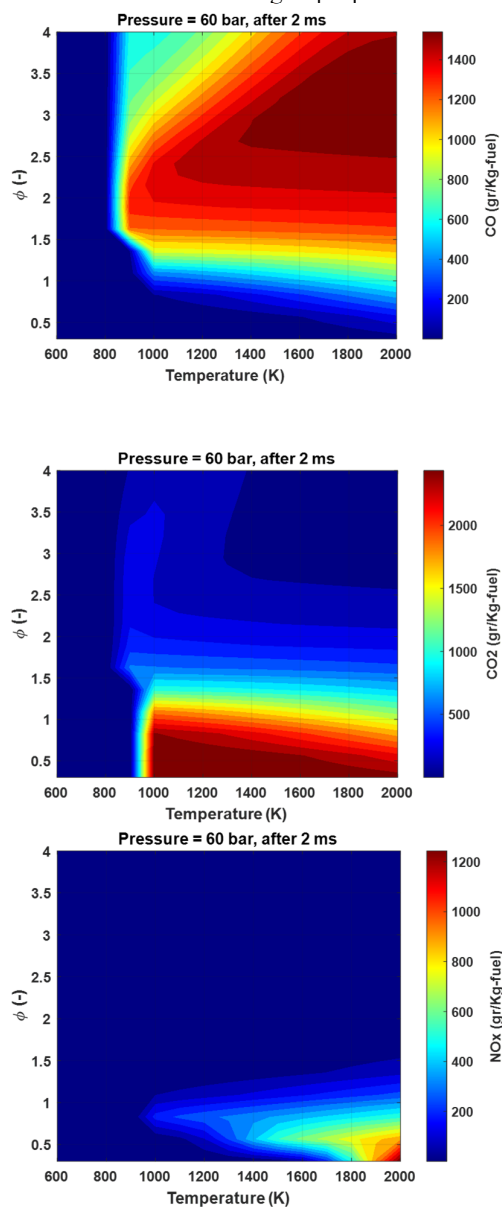

Fig.9 CO, CO2, NOx emissions obtained from homogeneous reactor simulation after 2ms for M42E21.

Conclusions

This work presented the validation of a kinetic mechanism consisting of 80 species and 349 reactions in a wide range of operating conditions for methanol, ethanol, iso-octane, and n-heptane. It has been shown that the model satisfactorily reproduces the ignition delay times and laminar flame speeds of all of the fuels. The validated mechanism was used to study and compare three different blends which have identical stoichiometric air to fuel ratio, volumetric energy content, octane numbers and latent heat in terms of combustion properties in both premixed and non-premixed configuration. The combustion and emissions properties of fuel blends were investigated. The results indicate ignition delay and laminar flame speed are more related to iso-octane and methanol content rather that ethanol. Generally, blends with lower iso-octane and higher methanol have led to longer ignition delay time and higher laminar flame speed. The main source of pollutant formation for one of the blends were also discussed.

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