Ignition delay times of ethanol-containing multi-component gasoline surrogates: Shock-tube experiments and detailed modeling

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ABSTRACT

Ignition delay times for binary (ethanol/iso-octane, 25%/75% by liquid volume) and quinary (iso-octane/toluene/n-heptane/diisobutylene/ethanol, 30%/25%/22%/13%/10%) gasoline surrogate fuels in air were measured under stoichiometric conditions behind reflected shock waves. The investigated post-shock temperature ranges from 720 to 1220 K at pressures of 10 bar for the binary mixture and 10 bar and 30 bar for the quinary mixture. Ignition delay times were evaluated using side-wall detection of CH* chemiluminescence (λ = 431.5 nm). Multiple regression analysis of the data indicates global activation energy of ~124 kJ/mol for the binary mixture and ~101 kJ/mol for the quinary mixture and a pressure dependence exponent of −1.0 was obtained for the quinary mixture. The measurements were compared to predictions using a proposed detailed kinetics model for multicomponent mixtures that is based on the reference fuels (PRF) model as a kernel and incorporates sub-mechanisms to account for the chemistry of ethanol, toluene and diisobutylene. The model was tested using the measured ignition delay times for the surrogate fuels. Additional comparisons are based on literature data for other fuel combinations of the single constituents forming the quinary surrogate to insure that the modified mechanism still correctly predicts the behavior of simple fuels. The proposed model reproduces the trend of the experimental data for all pure fuels and blends investigated in this work, including the pressure dependence.

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1. Introduction

With the development of improved combustion strategies for internal combustion engines and tailored fuels that are partially based on biomass-derived compounds, the need for an in-depth description of the fuel ignition chemistry is continuously increasing. Computational models that include a detailed chemical kinetics description are progressing rapidly to become important design and analysis tools in every field of combustion science and engineering [1]. Shock tubes allow to instantaneously heat up homogeneous air/fuel mixtures and therefore allow to isolate the effect of chemical kinetics on the ignition delay of fuel/air mixtures. The dependence of the ignition delay can be systematically studied as a function of fuel composition, pressure, temperature, and fuel/air equivalence ratio. Many researchers have made extensive use of shock tube measurements of ignition delay times in the development and validation of global and detailed kinetics models [2,3] for the ignition of pure hydrocarbons. Depending on the size of the hydrocarbon chain the number of possible chemical species

and reactions amount easily to hundreds or thousands. For instance, the kinetics model for pure iso-octane oxidation of Curran et al. [4] is composed by 857 chemical species allowing 3606 elementary reactions. For different pure fuels a different set of reactions and chemical species is required for the description of the reaction scheme. When different fuel components are mixed, the possibility of cross reactions among the different reaction intermediates typically requires to include additional chemical species and reactions. A typical gasoline consists of a mixture of hydrocarbons from C4 to C9 with small percentages of C10 and C11, distributed mainly among straight and branched alkanes, cycloalkanes, alkenes, cycloalkenes, and aromatics, with different additives [5]. Because practical fuels consist of hundreds of chemical species [6], the development of a full chemical kinetics mechanism for a real fuel is a problem intractable with current computational capabilities.

One way to address this modeling limitation is the development of surrogate fuels. These are defined as mixtures of a few pure compounds that match the physical and chemical characteristics of the target fuel [7]. Often, the surrogates contain one single representative species for the classes of hydrocarbon molecules present in the target fuel. The surrogate fuel is used both to develop a better understanding of the chemical behavior of the target fuel as well as an experimental model whose behavior can be reproduced

precisely at different laboratories, with different experimental methods and conditions. This work focuses on the high-pressure measurement and analysis of the shock-tube ignition delay time (IDT) of gasoline surrogates.

Pure components have been studied intensively. The ignition delay times (IDTs) of iso-octane, n-heptane and toluene have been investigated over different temperature–pressure experimental conditions in shock tube and some of them are reported in [8–12]. Studies of multi-components fuels are just appearing. Andrae et al. [13] reported autoignition data for four binary mixtures of gasoline surrogates involving PRF (primary reference fuel from heptane and iso-octane) and toluene (e.g., TRF, toluene reference fuel) covering RON and MON from 73.2 to 94, in a homogeneous charge compression ignition (HCCI) engine under different operating regimes. Yahyaoui et al. [14] measured the concentrations of the common intermediates and product species using a ternary and quaternary gasoline surrogate mixtures: iso-octane/toluene/1-hexene (50%/35%/15%, all mixture compositions given by ratios of liquid volume of the unmixed components), iso-octane/toluene/1-hexene/ETBE (47.5%/33.25%/14.25%/5%) and iso-octane/toluene/1-hexene/ETBE (45%/31.5%/13.5%/10%) in a jet-stirred reactor at atmospheric pressure, stoichiometric composition at 800–1130 K, and IDTs in a shock tube at 1310–1880 K, 2–10 bar, and equivalence ratios of 0.25–1.5. Fikri et al. [15] reported shock tube IDT measurements for ternary (n-heptane/iso-octane/ethanol, 18%/62%/20%) and quaternary (n-heptane/toluene/iso-octane/diisobutylene, 20%/45%/25%/10%) gasoline surrogates at 690–1200 K at 10, 30 and 50 bar and stoichiometric condition in air.

While there is a significant amount of data and models on single components, until recently, detailed kinetics models for multi-component fuels as gasoline surrogates were not available. Curran et al. [16] proposed the first detailed kinetics model for binary PRF mixtures at elevated pressures. The model was validated for the two components and their mixtures against experimental results from both a high-pressure flow reactor and a shock tube in the 550–850 K temperature range at 12.5 bar and in the 690–1220 K range at 40 bar, respectively. Good agreement between experimental results and simulation was achieved. Andrae et al. [13] reported a detailed kinetics model for the autoignition of primary reference fuels and n-heptane/toluene blends. This model was validated against experimental results from HCCI engines and shock tube IDTs. Recently, Andrae et al. [17] reported a semi-detailed kinetics model for ternary mixtures of PRF/toluene (i.e., TRF). The model was validated against shock tube data for mixtures of iso-octane/toluene/n-heptane (63%/20%/17%) and (69%/14%/17%) at stoichiometric conditions in air for 880–1150 K and 30 and 50 bar. Comparisons with rapid compression machine (RCM) data for an intake temperature of 318 K and an intake pressure of about 1 bar, RON numbers between 93.4 and 99.8 and equivalence ratios from 0.2 to 0.5 were performed as well. Similarly, Koshi et al. [18] reported a numerical study of the oxidation of TRF mixtures for a wide temperature and pressure including the effect of cross reactions between aromatic and aliphatic compounds. It was suggested that the reactions of alkene and aromatic radicals are the main steps controlling ignition.

Ethanol-based fuels, especially ethanol/gasoline blends with some other constituents such as diisobutylene, are increasingly being used to meet oxygenate requirements as well as the demands for new alternative fuels. In this context, we have recently reported experimental data and detailed kinetics models of some TRF fuels with and without ethanol [19]. The models were validated against shock tube data for a wide range of experimental conditions. The IDTs of the different gasoline surrogates were well predicted over a wide range of conditions, but the model showed weaknesses at low temperatures.

Recently, two works on detailed kinetics models for quinary mixtures as gasoline surrogate have been reported [20,21]. Both works included ethanol, iso-octane, n-heptane, diisobutylene, and toluene as surrogate fuels. Andrae [20] adapted his detailed model by combining it with the standard ethanol kinetics mechanism from Marinov [22], iso-octane and n-heptane base kinetics from Curran et al. [16], the toluene sub-mechanism from their previous work [23], and the diisobutylene (DIB) sub-mechanism from Metcalfe et al. [6]. The model was found to be sensitive to changes in temperature and pressure. In the same manner, Cancino et al. [21] took the ethanol mechanism from Marinov [22] and included an up-grade using the Konnov [24] model to account for oxidation of small hydrocarbons. Iso-octane and n-heptane base kinetics were taken from Curran et al. [16], the toluene mechanism from Andrae et al. [23] and Maurice [25], and the diisobutylene kinetics from Metcalfe et al. [6]. Both mechanisms do a good job although in [20] the low temperature is well predicted. It should be stated that in [20] the rate of many reactions in the DIB sub-mechanism were tuned to match the experimental IDTs.

In light of the impact of the different constituents forming a surrogate, there is a need to characterize the chemistry of the mixtures with models that still reproduce the behavior of the individual constituents. Therefore, the objective of this study is to propose a detailed kinetics model for a quinary gasoline surrogate containing ethanol (oxygenated hydrocarbon), iso-octane (iso-paraffin), n-heptane (n-paraffin), toluene (aromatic) and diisobutylene (olefin) and compare the predictions with new data at high pressure and previous data available in the literature for the individual components, binary, ternary and quaternary mixtures. The selected components cover the major hydrocarbon constituents of gasoline/ethanol blends.

This work combines two aspects: (i) It presents ignition delay data measured in shock tubes for binary and quinary mixtures that contain ethanol and (ii) it attempts to interpret these measurements based on current models and their combination.

2. Experiments

The experiments were carried out in the high-pressure shock tube at the University of Duisburg-Essen. This facility and the experimental procedures are described in earlier works [15,19, 26,27]. Gas mixtures were prepared by injecting liquid gasoline surrogate mixture into an evacuated, heated stainless-steel mixing vessel, with subsequent complete evaporation. The total amount of fuel mixture and the added air were controlled manometrically in order to ensure the desired equivalence ratio. The mixture was stirred for 60 min. All the experiments were performed with the shock tube, the mixing vessel and all connecting gas lines pre-heated to 50 °C. The shock speed was measured over two intervals using three piezo-electric pressure gauges. Pressure data were recorded with a time resolution of 0.1 μs. All ignition delay times shown in this work were determined by extrapolating the steepest increase of the CH* chemiluminescence emission (at 431.5 nm) signal to its zero level on the time axis as shown in Fig. 1. To account for cool flame appearance a second photo-multiplier (PMT) was operated to measure CH_2O chemiluminescence in the 400–450 nm wavelength range. The estimated uncertainty in reflected shock temperature is less than ±25 K. The experiments were carried out with synthetic air containing 79.5% N_2 and 20.5% O_2. The driver gas was mixed in situ by using two high-pressure mass-flow controllers. Helium was used as the main component and Argon was added to match the acoustic impedance of the test gas. Concentrations of 5 to 20% Ar in He were required to generate tailored shock waves.

Two gasoline surrogate mixtures were investigated in this work. A binary mixture composed by ethanol/iso-octane (25%/75% with RON/MON of 109/101) and a quinary mixture composed by
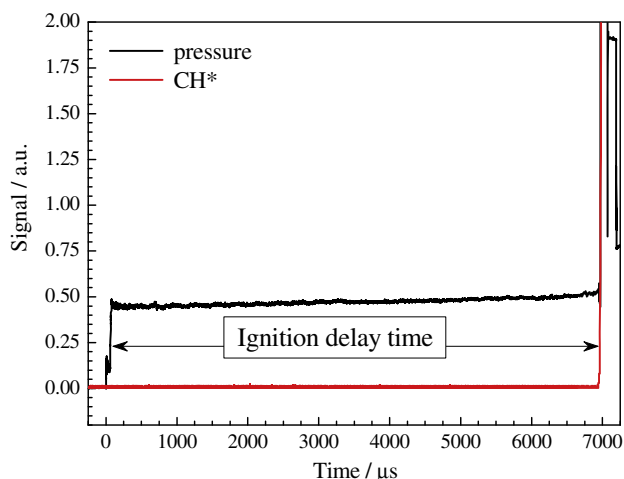
Fig. 1. Determination of the ignition delay time from the CH* chemiluminescence signal trace, quinary mixture at $p = 32.7$ bar, $T_5 = 720$ K and stoichiometric condition.

iso-octane/toluene/*n*-heptane/dib/ethanol (30%/25%/22%/13%/10% with RON/MON of 95.1/86.7). The RON/MON numbers of the mixtures were calculated using a SHELL program (Kalghatgi, G. Shell Global Solutions, Personal communication, 2008). The pure hydrocarbon fuels were obtained from Merck with a purity ⩾99.8%. A gas chromatographic analysis showed that Merck's 2,4,4-trimetylpentene (Merck, mixture of isomers – for synthesis) contained 70%/30% of the 1-pentene/2-pentene isomers, respectively.

3. Chemistry modeling

The adopted strategy for combining existing (sub-)mechanisms into a final detailed kinetics model has been described in earlier work [19,26,27]. It is based on merging available chemical kinetics substructures for each chemical species used in the surrogate mixture. When two chemical species have the same empirical formula, it is necessary to check their thermodynamic databases by comparing the enthalpy h, heat capacity c_p, and entropy s at several temperatures. If their thermodynamic properties return the same (or similar) values, then both chemical species are identical despite different names or abbreviations used in the original kinetics models. Then, one of the duplicated species is removed and the occurrences of that species are replaced by the equivalent one. Automatic mechanism checking is used to simplify the process.

In this work a detailed kinetics model for ethanol-based gasoline surrogates is proposed. Five chemical species were selected for which detailed oxidation chemistry is available in the literature and that are chemically representative for the main classes of hydrocarbons in a typical gasoline. The initial kinetics model that was tailored for the studied surrogates was the PRF model of Curran et al. [16]. This PRF mechanism, however, is not suitable for the description of lower molecular weight hydrocarbons (C1–C3) reactions. The chemical kinetics of ethanol oxidation was taken from Cancino et al. [26,28] which is an upgraded version of the ethanol-based Marinov [22] using Konnov's [24] mechanism, which is well validated for small hydrocarbons. The resulting mechanism was then combined with the toluene sub-mechanisms of Maurice [25] and Andrae et al. [23] and the sub-kinetics of diisobutylene were added from Metcalfe et al. [6]. The proposed detailed kinetics model for multicomponent ethanol-based gasoline surrogates is composed by 1130 chemical species allowing 5242 elementary reactions. The model is available in electronic format from the corresponding author.

4. Results and discussion

4.1. Measured ignition delay times

The measured IDTs (τ_{ign}) are listed in Table 1 along with the respective post-reflected-shock temperatures T_5, pressures p_5, and equivalence ratios ϕ for the two gasoline surrogate mixtures investigated experimentally in this work. At temperatures lower than those shown in Table 1 no ignition was observed within the test time of the experiment (15 ms). A regression analysis taking $\ln(\tau_{ign})$ as the dependent variable and $1000/T_5$ as the independent variable was performed for the binary mixture (ethanol/iso-octane) in the high temperature range (980–1200 K) and at 30 bar obtaining the apparent global activation of 124 ± 8 kJ/mol, as shown in Eq. (1).

$$\tau_{ign\ 30\ bar}/\mu s = 10^{-3.7 \pm 1.2} \exp\left(\frac{+124.8 \pm 23.7\ kJ/mol}{RT}\right) \quad (1)$$

Because the experiments for the binary mixture were only performed at 30 bar no estimate of the dependence on pressure is possible. For the quinary mixture (iso-octane/toluene/n-heptane/di-iso-butylene/ethanol), a regression analysis taking $\ln(\tau_{ign})$ as the dependent variable and $1000/T_5$ and $\ln(p)$ as the independent variables was performed in the high temperature range (980–1200 K), obtaining the apparent global activation of 101 ± 14.3 kJ/mol and a pressure dependence of -1.05, as shown in Eq. (2).

$$\tau_{ign}/\mu s = 10^{-1.1 \pm 0.81} \exp\left(\frac{+101.0 \pm 14.3\ kJ/mol}{RT}\right) p^{-1.05 \pm 0.3} \quad (2)$$

Table 1
Ignition delay times of the gasoline surrogate mixtures investigated in this work measured in the high-pressure shock tube.

ϕ	T_5 [K]	p_5 [bar]	τ_{ign} [μs]
Ethanol/iso-octane – 25%/75% by liquid volume			
1.0	1217	30.9	35
1.0	1215	30.8	34
1.0	1169	29.2	58
1.0	1164	30.7	74
1.0	1132	31.9	78
1.0	1059	30.6	404
1.0	1004	30.3	791
1.0	967	31.2	683
1.0	909	30.7	2039
1.0	862	31.1	2097
1.0	809	30.7	N–I
iso-octane/toluene/n-heptane/di-iso-butylene/ethanol – 30%/25%/22%/13%/10% by liquid volume			
1.0	1220	31.3	26
1.0	1156	27.6	122
1.0	1139	29.5	119
1.0	1100	30.0	204
1.0	1033	28.9	226
1.0	981	28.7	1010
1.0	928	28.3	1761
1.0	884	28.7	2734
1.0	884	33.1	2687
1.0	833	33.3	4176
1.0	779	33.2	4697
1.0	771	32.2	4625
1.0	721	32.7	6873
1.0	1243	10.8	120
1.0	1108	11.2	462
1.0	1067	9.3	834
1.0	1054	10.5	255
1.0	1010	10.2	1145
1.0	1002	11.3	1215
1.0	933	10.9	3563
1.0	869	10.5	N–I

N-I No ignition.

4.2. Numerical simulations

The proposed detailed kinetics model was compared to experimental results of IDTs of binary and quinary mixtures performed as a part of this work. Additional comparisons include experimental IDTs from literature for pure fuels, binary, ternary and quaternary mixtures of the various components of the quinary surrogate mixture to ensure that the merging of sub-mechanisms does not influence the prediction for single fuels and simple mixtures. A total of 401 numerical simulations were performed using the software CHEMKIN-PRO®. In this work we adopted the criterion of maximum oxygen atoms concentration as the ignition time. The results of the numerical simulation are presented in the following sections.

4.2.1. Pure fuels

Fig. 2 shows the numerical results of IDTs for stoichiometric mixtures of (a) ethanol/air, (b) iso-octane/air and (c) toluene/air. The detailed kinetics model captures the pressure dependence in the three reactive systems. It also agrees well with the trend of the experimental data. For ethanol the model underpredicts the IDT in the high temperature region. For iso-octane, the agreement with the measurements is relatively good. In Fig. 2c, for toluene, the measurements of Shen et al. [29] and Davidson et al. [12] were also included. The study in [29] was carried out for toluene/air mixture at 1021–1400 K, 10–61 bar, and ϕ = 1, 0.5, 0.25. It was found that the measured pressure versus time histories did not show significant pre-ignition energy release as it was noticed in the work of Davidson et al. [12]. The data from Shen et al. were scaled to the pressures of 17 and 47 bar by using their pressure scaling factor (-1.1). This was done because there were differences in the experimental prediction of IDTs for temperatures below 1100 K, pointed out by Shen et al. [29] as being a result of the influence of contamination in the Davidson's shock-tube experiments for toluene [12]. Note that the proposed detailed kinetics model agrees well with Shen's measurements for 47 bar, and in the high temperature range for 17 bar.

Fig. 2 also shows the simulation of the three individual reactive systems by using the respective kinetics base models for ethanol [28], PRF [16], and toluene [20]. For ethanol at lower temperatures the proposed multi-component model agrees well with the base model [28], while for higher temperatures the proposed model is slightly faster than the experiment underpredicting the IDTs by about ∼25%. For iso-octane, the proposed multi-component model shows faster ignition than the PRF model [16] in the temperature range investigated in this work. This effect is more evident for high temperatures. However, the low temperature range is better reproduced by the proposed multi-component model than the PRF model. For toluene, the multi-component model predicts IDTs that are shorter than the toluene base-model [23]. At high pressure the model of this work captures the behavior of the measurements better than that published in [23].

4.2.2. Binary mixtures

The results of the proposed detailed kinetics model were compared to measurements for two binary mixtures. Fig. 3a shows the numerical results for iso-octane/n-heptane (80%/20%, PRF80) compared to the measurements from [30,31], and Fig. 3b shows the experimental and numerical results of IDTs for iso-octane/ethanol (75%/25%) investigated in this work. For the PRF80 mixture, the proposed detailed kinetics model captures the IDTs well for temperatures higher than 850 K. For temperatures below 850 K, the experimental results show the typical Negative Temperature Coefficient (NTC) regime caused by the presence of n-heptane in the mixture. The simulation predicts the IDTs within an uncertainty of ∼20%. For the iso-octane/ethanol mixture (Fig. 3b), the simulation again agrees well with the experimental results within the uncertainty of the existing data. Fig. 3c shows the experimental
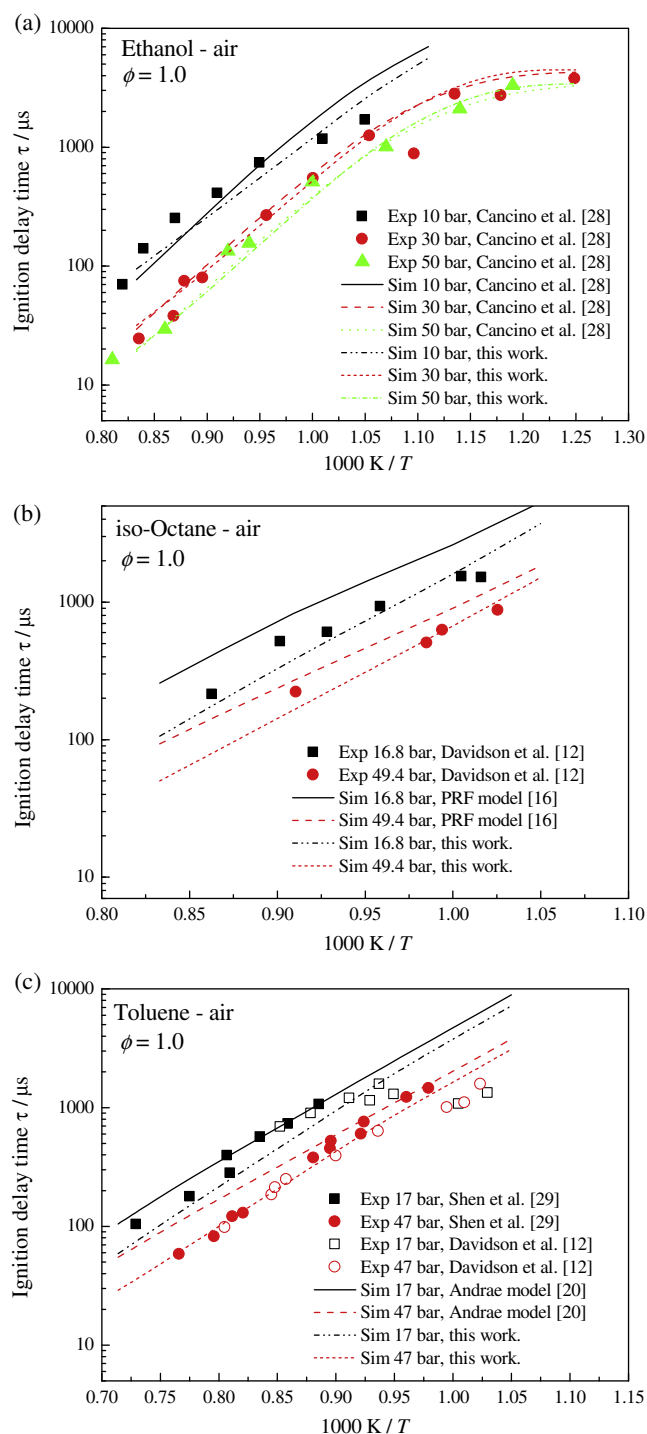

Fig. 2. Comparison of experimental and numerical results for the ignition delay time for pure fuels. Experimental data from literature, respective references given in the diagrams.

data from Fieweger et al. [31] (ϕ = 1.0 and pressure ∼40 bar) and the numerical prediction of IDT by using the PRF model and the detailed kinetics model for multi-component gasoline surrogates proposed in this work. It can be observed that the PRF model systematically overpredicts the IDT for all the experimental data of Fieweger et al. [31] and especially in the low temperature range (T < 1000 K). The proposed detailed kinetics model predicts the IDT better than the PRF model using the Fieweger's experimental data and both kinetics models are able to reproduce the NTC behavior as observed in Fig. 3c.
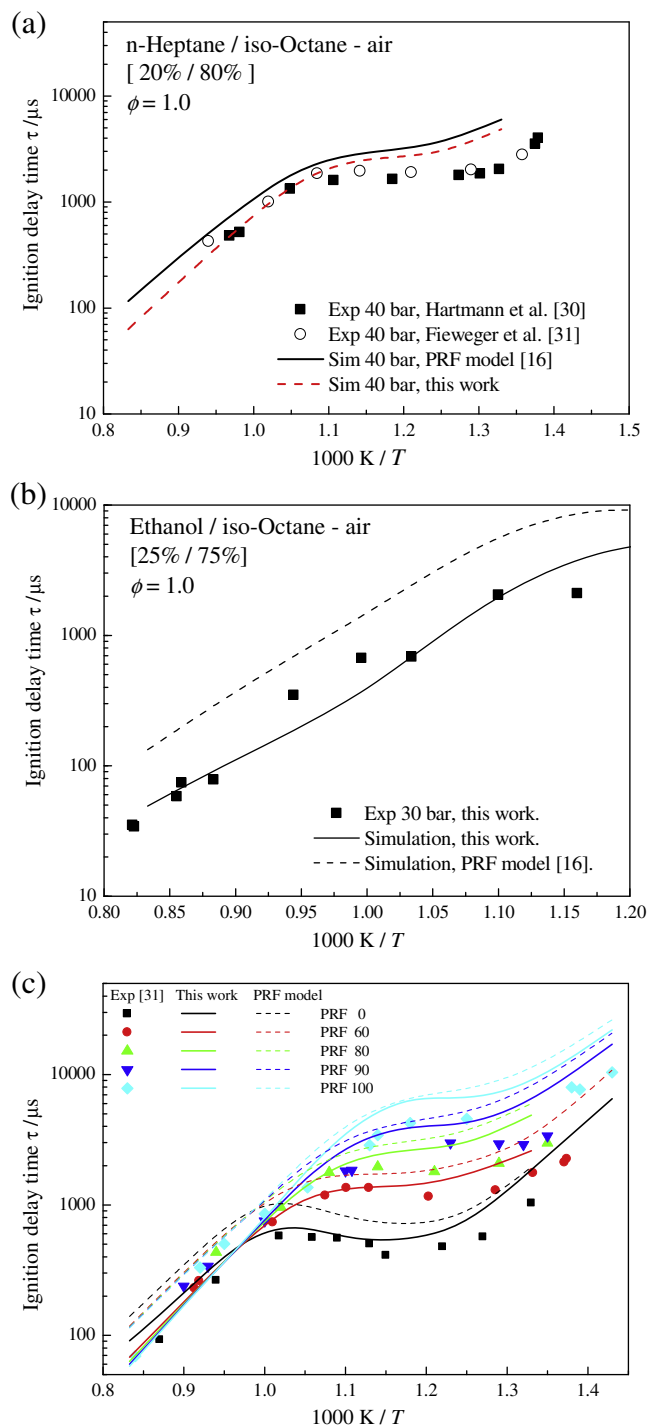
Fig. 3. Comparison of experimental and numerical results for the ignition delay time for binary mixtures.
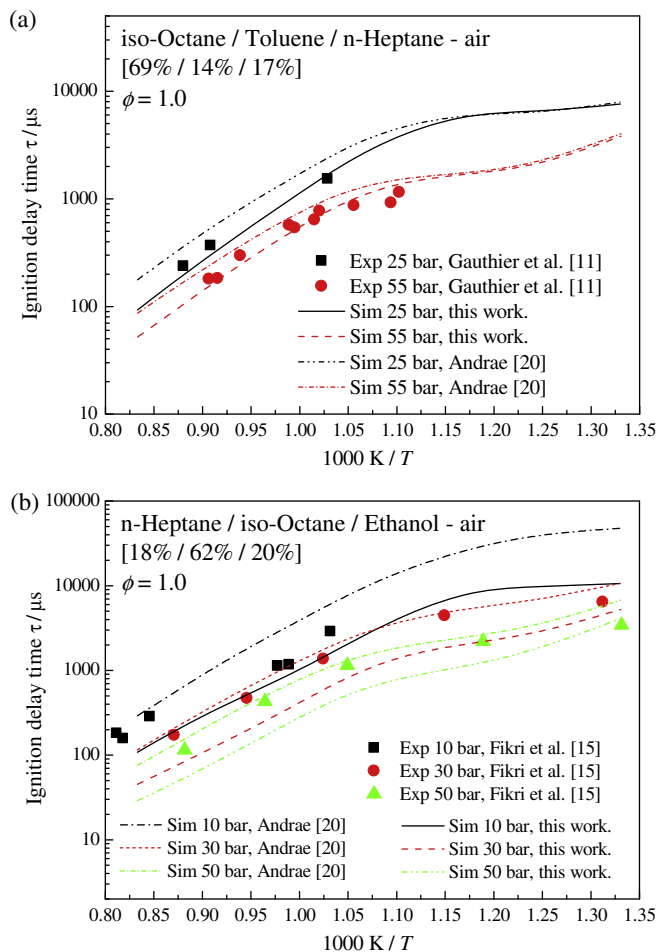

Fig. 4. Comparison of experimental (from Fikri et al. [15]) and numerical results for the ignition delay time for ternary mixtures.

proposed model predicts the change in slope in the 850–900 K temperature range for the Mix-a/air mixture at 55 bar. For the Mix-b/air mixture, the kinetics model provides IDTs that are shorter by a factor 2–3 compared to the measurement. Additionally, a comparison with the Andrae model [20] was also performed and is also shown in Fig. 4. It can be observed that for Mix-a the Andrae model slightly overestimates the ignition delay times especially at high temperature. For Mix-b, however, the Andrae model shows better agreement with the experimental results than our model.

4.2.4. Quaternary mixtures

Two additional experimental results of IDT based on quaternary mixtures [15,19] were also compared to the predictions of the proposed model. Fig. 5a compares simulated and measured IDTs for stoichiometric mixtures of toluene/iso-octane/n-heptane/di-iso-butylene (45%/25%/20%/10%) in air [15]. Again, the proposed model agrees well with the experimental results, capturing absolute values of IDT, and deviates from the experimental data for lower temperatures ($T < 780$ K) in the worst case only by about ~20%. Fig. 5a also shows the performance of the detailed kinetics model of Andrae [20]. It can be clearly seen that his model overpredicts the ignition delay time with a more pronounced deviation in the high temperature range. Fig. 5b shows the comparison of simulation and measurement for the stoichiometric mixture of ethanol/iso-octane/n-heptane/toluene (40%/37.8%/10.2%/12%) in air. Within the scatter of the experimental data the simulation gives satisfying results.
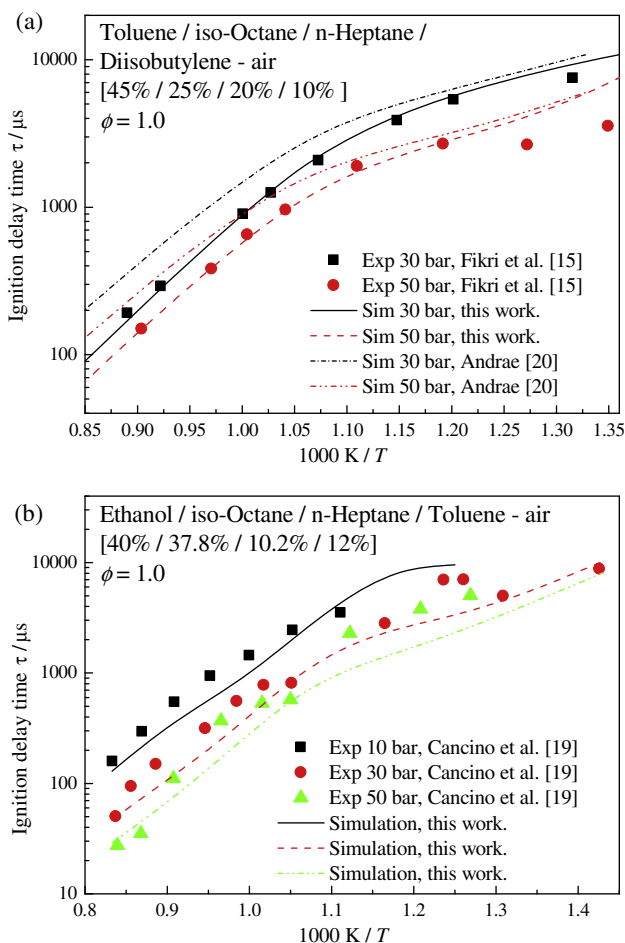
4.2.3. Ternary mixtures

Experimental IDT results available from the literature for two ternary mixtures were compared with the model predictions. Fig. 4 shows the comparison for the stoichiometric mixtures Mix-a (iso-octane/toluene/n-heptane, 69%/14%/17%) [11] and Mix-b (n-heptane/iso-octane/ethanol, 18%/62%/20%) [15] in air, respectively. The model from this work captures the pressure dependence for both ternary mixtures and agrees well with the experimental results from [11]. The proposed model deviates merely by ~15% from the experimental values. Furthermore, the

Fig. 5. Comparison of experimental (from Fikri et al. [15] and Cancino et al. [19]) and numerical results for the ignition delay time for quaternary mixtures.

Fig. 7. Sensitivity Coefficients of OH for the of the quinary mixture, with initial temperature of 1000 K, stoichiometric composition and pressure of 30 bar (Coefficients at 1290 K).

tions agree well with the experimental results representing the trend of the experimental data and capturing the pressure dependence, however, for the higher pressure, 30 bar, the model tends to underestimate the IDTs by about ~15%. Fig. 6 shows also the comparison of numerical and experimental results using the Andrae [20] model. The model of Andrae fails to predict the experimental values. The disagreement is as much as factor of ~2.2.

4.3. Sensitivity analysis

A sensitivity analysis based on the OH radical concentration for the quinary mixture was performed assuming a homogeneous reactor at the initial temperature of 1000 K, $\phi = 1$ and pressure of 30 bar. Fig. 7 shows the sensitivity coefficients for the eleven reactions having the highest sensitivities when the temperature increases to a value of 1290 K. From reaction flux analysis it can be deduced, that in the intermediate regime near to the ignition point, the hydroxyl radicals affect considerably the production/depletion of the parent fuels present in the mixture. Note, that in the intermediate temperature range, branching reactions are especially significant in enhancing the radical pool and hence in initiating ignition. Calculations showed that the most influential reaction is the H-abstraction of ethanol by the methylperoxy radical giving β-hydroxyethyl (SC$_2$H$_4$OH in the mechanism) and methyl peroxide ($C_2H_5OH + CH_3O_2 \Longleftrightarrow SC_2H_4OH + CH_3O_2H$). Additionally, the sensitivity analysis indicates the significance of the reaction of toluene with hydroxyl radical giving benzyl radicals ($C_6H_5CH_3 + OH \Longleftrightarrow C_6H_5CH_2 + H_2O$). The reaction of benzyl radicals with molecular oxygen competes with the reverse reaction of toluene with OH and therefore strongly affects the production of hydroxyl radicals. Finally, the hydroperoxide decomposition produces more OH radicals and promotes also the ignition.

5. Summary and conclusions

In this work, ignition delay times (IDTs) of binary (ethanol/iso-octane, 25%/75%, all percentages given by liquid volume prior to mixing) and quinary (iso-octane/toluene/n-heptane/diisobutylene/ethanol, 30%/25%/22%/13%/10%) gasoline surrogate mixtures

4.2.5. Quinary mixture

Shock-tube experiments were performed using a quinary mixture composed by iso-octane/toluene/n-heptane/diisobutylene/ethanol (30%/25%/22%/13%/10%). No experimental data for surrogate mixtures with more than four components were available in the literature so far. Fig. 6 shows the experimental and simulation results of IDT for the proposed quinary mixture. The model predicts
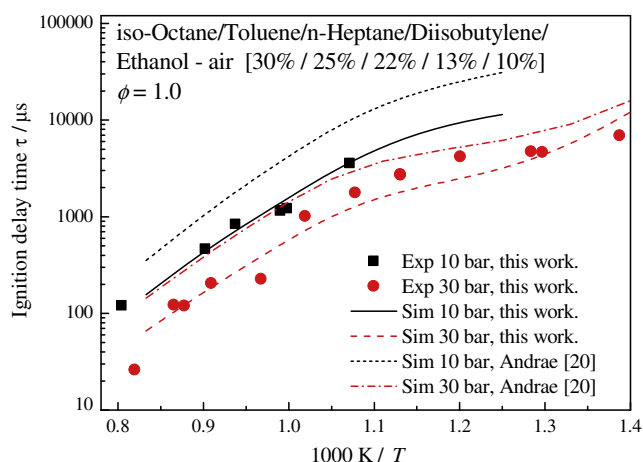

Fig. 6. Comparison of experimental and numerical results for the ignition delay time for a quinary mixture.
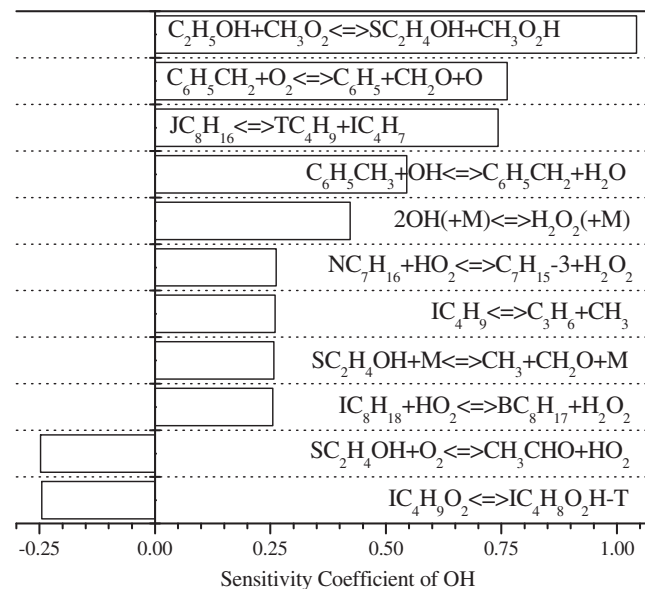
have been measured in the high-pressure shock tube facility at the University of Duisburg-Essen. The investigated post-reflected-shock temperatures were in the 720–1220 K range. The experiments were carried out at stoichiometric conditions at pressures of 10 bar for the binary mixture and 10 and 30 bar for the quinary mixture. IDTs were evaluated using side-wall detection of CH* chemiluminescence (λ = 431.5 nm). A detailed kinetics model for multi-component gasoline surrogate mixtures was proposed and compared against measurements of IDTs for pure fuels, binary, ternary quaternary and quinary mixtures as gasoline surrogates. The proposed detailed kinetics model was assembled by blending sub-mechanism schemes that are available in the literature for each component of the surrogate considered in this work. The results from the proposed model were compared to the predictions of the incorporated base-models for the pure fuels. The proposed model captures absolute values in the mixtures without ethanol and it underestimates IDTs for pure ethanol, mixtures containing ethanol, ternary, and quaternary mixtures. Nevertheless, the proposed model reproduces the trend of the experimental data for all pure fuels and blends investigated in this work, including the pressure dependence. Further reaction analysis of the predictions presented, as sensitivity and reaction path analysis, is recommended to further analyze the interplay among the different reaction paths during ignition in the shock tube. Also, further comparison to measurements with others gasoline surrogate mixtures with different proportions, at different pressures and equivalence ratios are necessary in order to further check the predictive capability of the proposed model in a wide range of conditions.

Acknowledgements

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