An experimental and modeling study of the shock tube ignition of a mixture of *n*-heptane and *n*-propylbenzene as a surrogate for a large alkyl benzene

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1. Abstract

Alkyl aromatics are an important chemical class in gasoline, jet and diesel fuels. In the present work, an *n*-propylbenzene and *n*-heptane mixture is studied as a possible surrogate for large alkyl benzenes contained in diesel fuels. To evaluate it as a surrogate, ignition delay times have been measured in a heated high pressure shock tube (HPST) for a mixture of 57% *n*-propylbenzene / 43% *n*-heptane in air ($\approx$21% O_2, $\approx$79% N_2) at equivalence ratios of 0.29, 0.49, 0.98 and 1.95 and compressed pressures of 1, 10 and 30 atm over a temperature range of 1000–1600 K. The effects of reflected-shock pressure and equivalence ratio on ignition delay time were determined and common trends highlighted. A combined *n*-propylbenzene and *n*-heptane reaction mechanism was assembled and simulations of the shock tube experiments were carried out. The simulation results showed very good agreement with the experimental data for ignition delay times. Sensitivity and reaction pathway analyses have been performed to reveal the important reactions responsible for fuel oxidation under the shock tube conditions studied. It was found that at 1000 K, the main consumption pathways for *n*-propylbenzene are abstraction reactions on the alkyl chain, with particular selectivity to the allylic site. In comparison at 1500 K, the unimolecular decomposition of the the fuel is the main consumption pathway.

2. Introduction

Current market diesel fuels predominantly contain a mixture of saturated hydrocarbons and high molecular weight aromatic compounds. To fully understand the reactivity of these fuels it is important to understand the chemistry of both of these classes of compounds. Diesel fuels contain hundreds of compounds in each of these chemical classes and it is not possible to develop a chemical kinetic model that simulates the chemistry of all of the components present. It is necessary to develop surrogate fuels comprising a smaller number of compounds which represent the chemical and physical properties of diesel fuel. Farrell *et al.* [1] identified *n*-decylbenzene as a possible diesel fuel surrogate component to represent the aromatic class in diesel fuel. To use *n*-decylbenzene as a surrogate diesel fuel, a detailed chemical kinetic mechanism needs to be developed and experimental data for its validation needs to be obtained. Unfortunately, it is difficult to study *n*-decylbenzene in shock tubes due to its extremely low vapor pressure. To circumvent this issue, we propose to create a surrogate for *n*-decylbenzene using a mixture of *n*-propylbenzene and *n*-heptane whose vapor pressures are adequate for shock tube investigations. The *n*-heptane and the alkyl side chain on *n*-propylbenzene would mimic the *n*-decyl side chain on *n*-decylbenzene and provide a fuel surrogate mixture that behaves like a large alkyl benzene. In this study we chose a mixture of 43% *n*-heptane and 57% *n*-propylbenzene, but it will be necessary to optimize the relative amounts of the two components to match a particular alkyl benzene component. Nevertheless, this mixture provides a good chemical kinetic model validation target for a large alkyl benzene surrogate.

A number of studies have been performed on the single component fuels *n*-propylbenzene and *n*-heptane. We first review the *n*-propylbenzene studies. Litzinger *et al.* used a plug-flow reactor to study its oxidation at 1 atm pressure, at a temperature of approximately 1060 K and at equivalence ratios of 0.65, 1.0 and 1.5 highly diluted in nitrogen (99%) [2].

Roubaud *et al.* carried out rapid compression machine experiments on eleven different alkylbenzenes (including *n*-propylbenzene) in the lower temperature region (600–900 K), at compressed pressures of up to 25 bar for stoichiometric mixtures in air [3, 4].

Dagaut *et al.* [5] carried out experiments in a jet-stirred reactor (JSR) on *n*-propylbenzene oxidation at atmospheric pressure over a temperature range of 900–1250 K at atmospheric pressure and at equivalence ratios of 0.5, 1.0 and 1.5 highly diluted in nitrogen (≥ 50 ppm of O_2 and H_2O; ≥ 1000 ppm of Ar; ≥ 5 ppm of H_2). These experiments provided concentration versus temperature profiles of 23 different species. In addition, they developed a kinetic reaction mechanism for the oxidation of *n*-propylbenzene containing 124 species and 985 reactions.

A recent study by Gudiyella and Brezinsky [6] on *n*-propylbenzene produced high-pressure single-pulse shock tube speciation data obtained at shock pressures of 25 and 50 atm, at temperatures between 838–1669 K and equivalence ratios between 0.5–1.9. Species concentration versus temperature data for a variety of stable species was reported. A kinetic model has also been reported in this study.

Darcy *et al.* [7] measured ignition delay times in a heated high pressure shock tube for mixtures of *n*-propylbenzene in air at equivalence ratios of 0.29, 0.48,

0.96 and 1.92 and at reflected shock pressures of 1, 10 and 30 atm in the intermediate–to–high temperature regime (1000–1600 K). A comparative study with *n*-butylbenzene was also performed at these conditions, with both alkyl benzenes showing very similar reactivity. Moreover, a detailed chemical kinetic mechanism was used to simulate this data. This mechanism was based on that published for *n*-propylbenzene oxidation and subsequently modified for *n*-butylbenzene oxidation in a jet-stirred reactor at 10 atm under dilute conditions over the temperature range 550–1180 K and at equivalence ratios of 0.25, 0.5, 1.0 and 2.0 by Diévart and Dagaut [8].

With respect to studies on *n*-heptane, its ignition behavior has been investigated extensively as a primary reference fuel and as part of a surrogate fuel mixture to represent larger fuels [9, 10, 11, 12, 13].

This study will provide ignition delay time measurements in the high temperature regime (1000–1600 K) for the *n*-propylbenzene and *n*-heptane surrogate measured in the heated high pressure shock tube (HPST) facility at NUI Galway. These experimental data are used to validate a combined chemical kinetic mechanisms for *n*-propylbenzene and *n*-heptane which can be used as a surrogate for *n*-decylbenzene, a diesel fuel surrogate component.

3. Experimental

3.1. Apparatus

Ignition delay times were measured in a high-pressure shock tube consisting of a stainless steel tube of 8.76 m in length, with an internal diameter of 6.3 cm. A double-diaphragm section divides the shock tube into a 3 m long driver section

and a 5.73 m driven section. Polyethylene terephthalate films (KATCO) were used as diaphragms in all experiments, where the thickness of the diaphragm material was chosen depending on the desired final shock pressure and varied from 75–500 μm. The driver gas used was helium (99.99% pure; BOC). The operational pressure limit of the shock tube is approximately 60 bar. The diagnostic system involves four pressure transducers, where the velocity of the incident shock wave was measured at three locations separated by known distances with the shock velocity extrapolated to the endwall. The pressure at the endwall was monitored using a pressure transducer (PCB, 113A24). The incident shock velocity at the endwall was used to calculate the temperature and pressure of the mixtures behind the reflected shock wave using the equilibrium program Gaseq [14].

The ignition delay time was defined as the interval between the rise in pressure due to the arrival of the shock wave at the endwall and the maximum rate of rise of the pressure signal. Pressure traces were obtained using a Sigma digital oscilloscope (Sigma, 90–4), with typical pressure trace shown in Fig. 1. Any experiments exhibiting significant pre-ignition pressure rise ($\geq$5% / ms) were excluded from the study in an attempt to minimize any non-ideal effects, in order for the data to be accurately simulated by assuming constant volume and homegeneous adiabatic conditions behind the refelcted shockwave.

Estimated uncertainty limits of the measurements are $\pm$ 15 K in reflected shock temperature, T_5, $\pm$ 15% in ignition delay time, τ, and $\pm$ 10 % in mixture composition.

A heating system was designed and installed on the driven section and man-

ifold of the shock tube to ensure that the vapor pressure of *n*-propylbenzene was well below the saturation vapor pressure (0.5 kPa at $25°C$ [15]) for the duration of the experiment and that no condensation of the fuel occurred. This heating system was described in detail in a previous paper [7].

Mixtures were prepared using direct injection of the liquid fuel into heated mixing vessels using a 5 ml gas-tight syringe (SGE Analytical Science, 008760). The partial pressure of fuel was measured using an MKS pressure transducer and digital readout followed by the addition of oxygen and nitrogen to a final known pressure.

n-Propylbenzene was supplied by Tokyo Chemicals Ltd. ($\geq$ 99% purity GC grade). Oxygen ($\geq$ 99.5% purity) and nitrogen ($\geq$ 99.998% purity) were supplied by BOC Ltd. Table 1 describes the reactant compositions examined in this study.

4. Results and discussion

4.1. Chemical kinetic model

The detailed chemical kinetic mechanism used in this study has been derived from Dagaut *et al.* [5] for *n*-propylbenzene oxidation. The mechanism, including 404 species and 2210 reactions, has been updated by Darcy *et al.* [7] to improve shock tube ignition predictions by substituting the original C_0–C_4 chemistry with the recently updated version from the Combustion Chemistry Centre at Galway [16] and introducing new pressure dependent unimolecular decomposition rates for *n*-propylbenzene. The C_0–C_4 sub-mechanism is based on our previous work [17, 18, 19], with the most recent updates described in [20, 21]. The chem-

istry of some important unsaturated species including 1,3-butadiene, propene and allene are taken from Laskin *et al.* [22], primarily based on the earlier work of Davis *et al.* [23].

Further modifications also included newly estimated abstraction reaction rate constants for the secondary benzyl hydrogen by $\dot{H}$, $\dot{O}H$, $H\dot{O}_2$, $\dot{C}H_3$, and $CH_3\dot{O}$ radicals and O_2 which were assigned to match the rates adopted in the base chemistry for abstraction reactions on secondary allylic hydrogens [7]. The resulting mechanism captures the ignition delay measurements over a broad range of conditions maintaining the agreement with the JSR experiments by Dagaut *et al.* [5] in the same way as presented by Darcy *et al.* [7]. In order to simulate the combustion behavior of a *n*-heptane/*n*-propylbenzene mixture, this mechanism has been merged with the *n*-heptane mechanism of Mehl et al. [24]. The mechanism and thermochemistry files are included as Supplemental Material.

Further modifications were made to the combined mechanism in the present study. Abstractions from the primary (methyl group) and secondary site (next to the methyl) on *n*-propylbenzene were set to match the reaction rate constants for these types of reactions used in the base chemistry (C_1–C_4 module). The benzyl plus $H\dot{O}_2$ reaction leading to the formation of the benzoxy and $\dot{O}H$ radicals has been set to 1×10^{13} cm^3 mol^{-1} s^{-1} following the recommendation of Metcalfe *et al.* [25].

Beta-decomposition reactions of the phenyl-propyl radicals were also updated, writing them in the exothermic direction which represents the addition of a radical to an alkene moiety. Reaction rate constants for analogous reactions from Mehl

et al. [26] were adopted, except in the case of the addition of the phenyl radical to propene which was derived from Park *et al.* [27]. Reactions were added to account for the formation of the *n*-propenylbenzene: Hydrogen elimination from the phenyl-propyl radicals (active at high temperature) and O_2 addition on the phenyl-propyl radicals followed by concerted $H\dot{O}_2$ elimination (active at low temperature). Reaction rates for these reactions were taken from analogous reaction in the mechanism of 1-pentene by Mehl *et al.* [26]. The abstraction reaction of hydrogen by oxygen molecules from the allylic site of cyclopentadiene has been set to be the same as analogous reaction on the allylic site on n-propylbenzene.

Finally, the cross reactions allowing the hydrogen transfer between *n*-heptane and *n*-propylbenzene radicals have been included as previously done for *n*-heptane / toluene mixtures [24].

The resulting mechanism includes about 900 species and 4160 reactions and is available as supplemental data. The thermodynamic data for the *n*-propylbenzene species was the same as in [7] while the thermodynamic data from the *n*-heptane mechanism was the same as in [24] , except three phenyl-propylperoxy radicals computed by THERM [28] and added to the database.

The detailed kinetic mechanism presented has been used to simulate the ignition delay times of a 57% *n*-propylbenzene / 43% *n*-heptane mixture using Chemkin-Pro [29] assuming adiabatic, constant volume conditions with no inhomogeneities.

4.2. Large alkyl benzene surrogate oxidation results

The results obtained for the oxidation of the large alkyl benzene surrogate are shown below. All experimental results can be found in the Supplemental Material.

4.2.1. Effect of pressure on ignition delay time

The effect of pressure on ignition delay times on a surrogate for large alkyl benzene oxidation was studied at four equivalence ratios (0.29, 0.49, 0.98 and 1.95). Ignition delay times of the surrogate versus inverse temperature at the various equivalence ratios and at pressures of 1, 10 and 30 atm are shown in Fig. 2. The model shows good agreement across the whole temperature and pressure space covered by the experiments, with the exception of the low pressure condition at fuel rich and stoichiometric conditions where the model predicts increasingly slow ignition delay times for the lowest temperatures studied. For both the measurements and simulations, an increase in pressure leads to an increase in reactivity (or a decrease in the ignition delay times) for all equivalence ratios studied. These results are typical of the effect of pressure on ignition delay time, for example [30].

4.2.2. Effect of fuel on ignition delay time

Figure 2 also shows the effect of the composition of the fuel influences reactivity. To investigate this simulations were carried out using the mixtures described above (represented by the solid lines), *n*-propylbenzene (represented by the dashed line) and *n*-heptane(denoted by the dotted line) at the same pressure, equivalence ratio and temperature. From these results it can be seen that in general

the reactivity is controlled by the alkane segment (*n*-heptane) with the exception of the lowest temperatures studied at low pressures where *n*-propylbenzene seems to have greater control over the reactivity of the fuel. This indicates that the alkyl chain length of these large alkyl aromatic compounds defines their reactivity.

4.2.3. Effect of equivalence ratio on ignition delay time

The effect of equivalence ratio on ignition delay times was determined by measuring ignition delay times at four fuel/air mixture compositions at 10 and 30 atm, Fig. 3. Again,the model shows reasonably good agreement across the whole temperature and stoichiometry space covered by the experiments.

Starting first with the results at 10 atm, the reactivity of all equivalence ratios at 10 atm is very similar and much of the data could be described as being the same within the uncertainty of the experimental data over this temperature range (975–1481 K), Fig. 3a. If one looks closely at the data however and uses the model predictions as a guide, it can be noted that richer conditions react faster than leaner at the lowest temperatures studied (1000–1100 K). The rest of the temperature range shows a convergence of data at all equivalence ratios and indicates that equivalence ratio does not play a key role in reactivity from 1100 to 1400 K, Fig. 3a.

At 30 atm, Fig. 3b, the entire temperature range studied (1000-1360 K) seems to be exhibiting intermediate temperature chemistry as fuel-rich mixtures react fastest and fuel-lean mixtures have the lowest reactivity. This behavior at slightly lower temperatures is attributed to the chain branching sequence $RH + H\dot{O}_2 = \dot{R} +$

H_2O_2 followed by $H_2O_2 + M = \dot{O}H + \dot{O}H + M$, where RH is the fuel components. In the present experiments, the equivalence ratio is increased by increasing the fuel concentration ([RH]) which enhances the rate of this branching sequence that produces two reactive $\dot{O}H$ radicals. Once again at the highest temperatures studied, a convergence of the data is beginning to occur which would indicate that high temperature chemistry is beginning to take over the system but a clear view of this is not possible as the fuel is so reactive it is impossible to accurately determine the ignition delay time as it becomes too short ($\leq 30\ \mu$s). From here it can be seen that the crossover from high- to intermediate-temperature chemistry occurs at increasing temperatures with increasing reflected shock pressures. These results are consistent with those observed for *n*-propylbenzene in a previous study [7].

4.3. Sensitivity and reaction pathway analysis

4.3.1. Reaction path analysis

The detailed mechanism can be used to analyze the chemistry controlling the autoignition behavior of the mixture. In order to achieve a better understanding of reactions consuming the fuel and intermediate products, and the interactions between the two mixture components, a reaction path analysis has been carried out at 10 atm, $\phi = 1.0$, 1000 K and 1500 K, and 10% fuel consumed, these being most representative for the experimental conditions studied.

In the path analysis (Fig. 4), we focus attention on the aromatic component, since *n*-heptane has already been discussed in previous publications (e.g. [11]).

At 1000 K (bold percentages), the main consumption pathways for *n*-propyl-

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benzene are abstraction reactions on the alkyl chain, mainly by $\dot{O}H$ radicals. A strong selectivity on the ethyl-benzyl (allylic) site is observed, accounting for about the 50% on the total abstraction rate. The primary site (designated by A in the species PBZjA), is the least targeted by abstraction and, due to the weakness of the allylic C–C bond in PBZjA formed, it rapidly decomposes to benzyl radicals and ethylene. For the same reason, the homolythic decomposition of the fuel to benzyl and ethyl radicals is observed as a relevant consumption pathway even at this relatively low temperature of 1000 K.

When the abstraction occurs on the secondary site (forming PBZjB), the radical is mainly consumed via the O_2 addition/concerted $H\dot{O}_2$ elimination pathway, showing a selectivity of 2:1 toward the formation of 2-propenylbenzene versus 1-propenylbenzene, new paths added to the current mechanism.

The predominant ethylbenzyl radicals (labeled as PBZjC), are mostly consumed via reaction with $H\dot{O}_2$ radicals leading to the formation of benzaldehyde and $\dot{O}H$ and ethyl radicals. Because of the intrinsic stability of the ethyl benzyl radicals, the O_2 addition step leading to $H\dot{O}_2$ radical elimination is less favored than a secondary site, and only 20% of the initial PBZjC formed follows this pathway, an amount comparable with its decomposition to $\dot{C}H_3$ radical and styrene.

At high temperature (1500 K, italic percentages), the unimolecular decomposition of the fuel dominates and abstraction reactions (now mostly involving $\dot{H}$ atoms) are far less selective, attacking at a similar rate at all the three sites on the alkyl chain (1000 K: PBZjA/PBZjB/PBZjC 17/29/54%, 1500 K: PBZjA/PBZjB/PBZjC 25/35/40%). Abstraction reactions are followed by beta-decompositions lead-

ing primarily to ethylene and benzyl radicals, styrene and $\dot{C}H_3$ radicals and 1-propenylbenzene and $\dot{H}$ atoms.

4.3.2. Sensitivity analysis

Using Chemkin Pro, the sensitivity of $\dot{O}H$ radical concentration to different reaction rate constants was computed at the same conditions as the reaction path analysis (Fig. 5). Independent of temperature, the initiation step leading to benzyl plus ethyl radicals promotes the reactivity of the system. At 1500 K, the ethyl radical rapidly decomposes to ethylene and a $\dot{H}$ atom and this reaction exhibits a high sensitivity. At 1000 K, where the reactivity is controlled by $\dot{O}H$ and $H\dot{O}_2$ radicals, the benzyl radical, together with the ethyl benzyl (PBZjC) radical assist the conversion of relatively un-reactive $H\dot{O}_2$ radicals to reactive $\dot{O}H$ radicals, promoting reactivity. Also, $H\dot{O}_2$ radicals react with *n*-propylbenzene at the benzyl site and with *n*-heptane on the secondary sites, producing H_2O_2 which decomposes into two $\dot{O}H$ radicals, enhancing the reactivity of the system. The latter steps are the most important reactions involving *n*-heptane which promote the overall reactivity of the fuel mixture. Since this is a fuel mixture, cross reactions (e.g. *n*-C_7H_{16} + benzyl radical) are of interest, but they did not appear as being important in the sensitivity analysis.

5. Conclusions

This study presents a comprehensive experimental and modeling study of the shock tube ignition of a surrogate fuel for large alkyl benzenes, consisting of 57%

n-propylbenzene and 43% *n*-heptane, over the temperature range of 1000–1700 K, equivalence ratios of (0.29, 0.49, 0.98, and 1.95), and reflected shock pressures of (1, 10 and 30 atm).

It was found that an increase in reflected shock pressure resulted in shorter ignition delay times for all equivalence ratios investigated. Experiments and simulations on the effect of equivalence ratio on ignition delay time showed fuel-rich mixtures were most reactive at lower temperatures, while at higher temperatures the reactivity of all equivalence ratios was very similar. The influence of equivalence ratio at lower temperatures was attributed to the chain branching sequence of $RH + H\dot{O}_2 = \dot{R} + H_2O_2$ followed by $H_2O_2 + M = \dot{O}H + \dot{O}H + M$, where RH is the fuel.

The kinetic reaction mechanism by Diévart and Dagaut [8] was updated and used to simulate the experimental data. The simulations showed very good agreement with the experimental ignition delay and captures the trends in pressure, temperature and equivalence ratio well.

Reaction path analysis showed that the *n*-propylbenzene was mainly consumed at 1000 K by $\dot{O}H$ radicals through $\dot{H}$ atom abstraction at the benzylic site. At 1500 K, *n*-propylbenzene was mainly consumed through unimolecular decomposition reactions. The sensitivity analysis showed that the specific decomposition reaction leading to benzyl and ethyl radicals was promoted the system's reactivity at all temperatures. Further theoretical and experimental investigations are needed to obtain a more accurate rate constant for this important reaction. At 1000 K, the reactivity is mainly controlled by reactions involving $H\dot{O}_2$ and $\dot{O}H$ radicals, with

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the $H\dot{O}_2$ and benzyl reaction being particularly important. To fully cover the range of conditions found in a diesel engine, further autoignition experiments are needed at lower temperatures to validate the chemical kinetic mechanism.

6. Acknowledgments

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7. List of Supplemental Materials

* Chemical kinetic mechanism (CHEM.mech)

* Thermodynamic data (THERM.dat)

* Experimental data (Expt_data.pdf)

* *n*-propylbenzene paper previously submitted (included for reference for reviewers) (npropylbenzene_paper(for_reference).pdf)
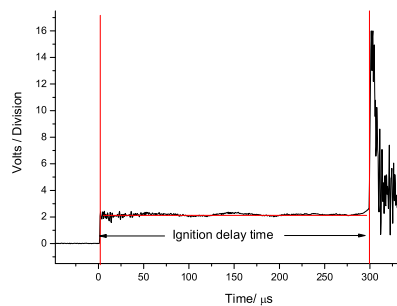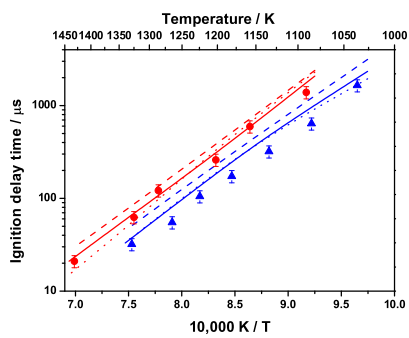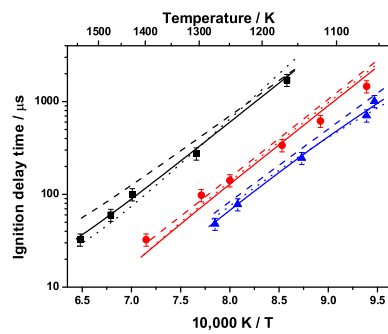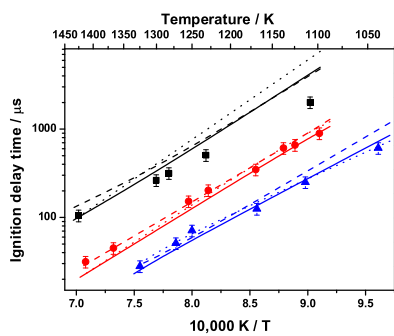
8. List of figure captions

1: Typical pressure trace of *n*-decylbenzene surrogate oxidation; $\phi = 0.29$ (0.30% *n*-propylbenzene, 0.23% *n*-heptane), $p_5 = 27.82$ atm, $T_5 = 1181$ K, Ignition delay time = 173 μs

2: Effect of varying reflected shock pressure on the reactivity of a large alkyl benzene surrogate ; ▪– 1 atm, ●– 10 atm, ▲– 30 atm. Symbols are experimental data, —— mixture model predictions, – – – *n*-propylbenzene model predictions, · · · *n*-heptane model predictions.

3: Effect of varying equivalence ratio (ϕ) on the reactivity of a large alkyl benzene surrogate; ▪– $\phi = 0.29$, ●– $\phi = 0.49$, ▲– $\phi = 0.98$, ▼– $\phi = 1.95$. Symbols are experimental data, lines are model predictions.

4: Reaction path analysis of *n*-propylbenzene in the oxidation of *n*-heptane/ *n*-propylbenzene mixtures at 10 atm, $\phi = 1.0$ at 10% conversion of *n*-propylbenzene: bold numbers: 1000 K, italic numbers 1500 K. The numbers represent the percent of fuel flux that goes through a particular species.

5: Sensitivity analysis on $\dot{O}H$ radical formation in the oxidation of *n*-heptane / *n*-propylbenzene mixtures at 10 atm, $\phi = 1.0$ and 10% conversion of the fuel

9. Tables

Table 1: Molar composition of surrogate mixtures

ϕ^a	% n-propylbenzene	% n-heptane	O_2	% N_2
1.95	1.95	1.47	20.32	76.43
0.98	0.99	0.75	20.65	77.70
0.49	0.50	0.38	20.83	78.34
0.29	0.30	0.23	20.89	78.61

[a] *ϕ relates to the fuel/ air ratio*

10. Figures

Figure 1: Typical pressure trace of *n*-decylbenzene surrogate oxidation; ϕ = 0.29 (0.30% *n*-propylbenzene, 0.23% *n*-heptane), p_5 = 27.82 atm, T_5 = 1181 K, Ignition delay time = 173 μs
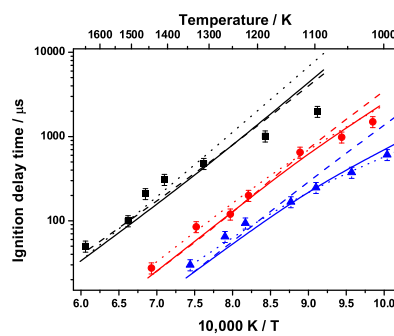
(a) $\phi = 0.29$
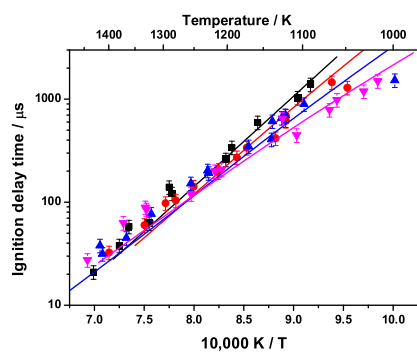
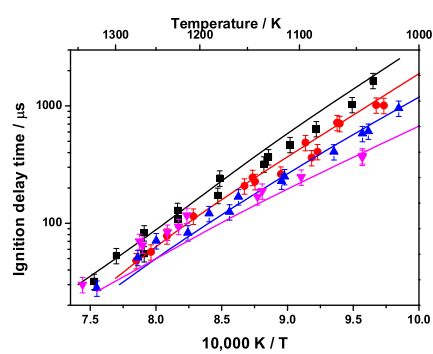(b) $\phi = 0.49$

(c) $\phi = 0.98$

(d) $\phi = 1.95$

Figure 2: Effect of varying reflected shock pressure on the reactivity of a large alkyl benzene surrogate ; ■– 1 atm, ●– 10 atm, ▲– 30 atm. Symbols are experimental data, —— mixture model predictions, – – – n-propylbenzene model predictions, $\cdots$ n-heptane model predictions.

(a) p_5 = 10 atm

(b) p_5 = 30 atm

Figure 3: Effect of varying equivalence ratio (ϕ) on the reactivity of a large alkyl benzene surrogate; ■– ϕ= 0.29, ●– ϕ= 0.49, ▲– ϕ= 0.98, ▼– ϕ= 1.95. Symbols are experimental data, lines are model predictions.
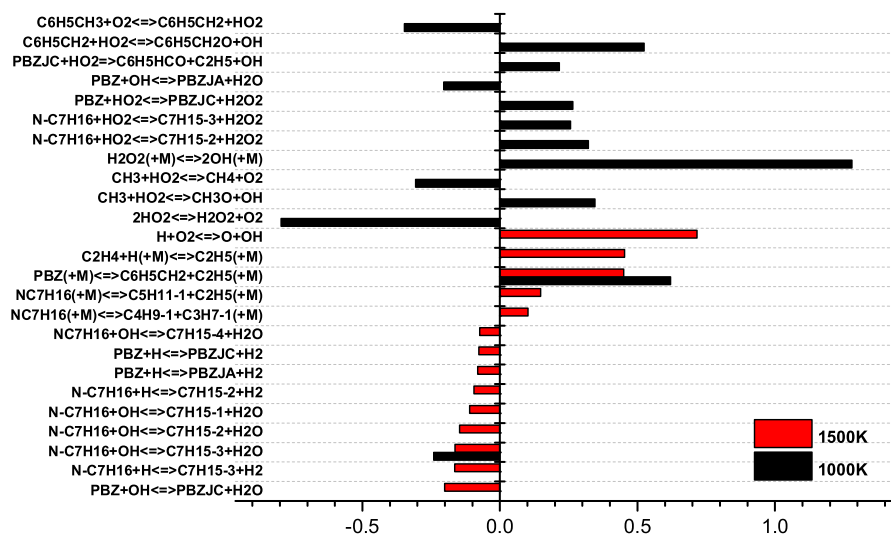
Figure 4: Reaction path analysis of *n*-propylbenzene in the oxidation of *n*-heptane / *n*-propylbenzene mixtures at 10 atm, ϕ= 1.0 at 10% conversion of *n*-propylbenzene: bold numbers: 1000 K, italic numbers 1500 K. The numbers represent the percent of fuel flux that goes through a particular species.

Figure 5: Sensitivity analysis on ȮH radical formation in the oxidation of *n*-heptane / *n*-propylbenzene mixtures at 10 atm, ϕ= 1.0 and 10% conversion of the fuel

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