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## Mixed butanols addition to gasoline surrogates: Shock tube ignition delay time measurements and chemical kinetic modeling

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## ABSTRACT

The demand for fuels with high anti-knock quality has historically been rising, and will continue to increase with the development of downsized and turbocharged spark-ignition engines. Butanol isomers, such as 2-butanol and tert-butanol, have high octane ratings (RON of 105 and 107, respectively), and thus mixed butanols (68.8% by volume of 2-butanol and 31.2% by volume of tert-butanol) can be added to the conventional petroleum-derived gasoline fuels to improve octane performance. In the present work, the effect of mixed butanols addition to gasoline surrogates has been investigated in a high-pressure shock tube facility. The ignition delay times of mixed butanols stoichiometric mixtures were measured at 20 and 40 bar over a temperature range of 800–1200 K. Next, 10 vol% and 20 vol% of mixed butanols (MB) were blended with two different toluene/n-heptane/iso-octane (TPRF) fuel blends having octane ratings of RON 90/MON 81.7 and RON 84.6/MON 79.3. These MB/TPRF mixtures were investigated in the shock tube conditions similar to those mentioned above. A chemical kinetic model was developed to simulate the low- and high-temperature oxidation of mixed butanols and MB/TPRF blends. The proposed model is in good agreement with the experimental data with some deviations at low temperatures. The effect of mixed butanols addition to TPRFs is marginal when examining the ignition delay times at high temperatures. However, when extended to lower temperatures ( $T < 850$  K), the model shows that the mixed butanols addition to TPRFs causes the ignition delay times to increase and hence behaves like an octane booster at engine-like conditions.

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### 1. Introduction

Over the last few decades, spark-ignition (SI) engines have encountered great improvements in fuel economy and emissions, driven by stringent environmental regulations [1]. The automotive industry has worked extensively to develop engines that utilize existing fuels (e.g., gasoline), while increasing the engine performance and durability. This development is expected to continue according to future projections, which anticipate a movement towards reducing fuel consumption of SI engines through downsizing and turbocharging (i.e., boosting) [2–4]. Downsizing and turbocharging can improve engine thermal efficiency by reducing throttling losses, as the engine will operate mostly at full throttle. Also, the downsized engine has lower weight and volume causing the frictional (mechanical) losses to decrease. In addition, the engine is expected to operate at higher loads due to turbocharging, which also contributes to improve the

overall efficiency of the engine. However, pursuing such technologies requires fuels with more resistance to auto-ignition because the high-load operating conditions of the engine will potentially increase the possibility engine knock [5,6]. Therefore, knock occurrence is the major constraint that prevents SI engines from reaching their full potential.

Kalghatgi [5,6] defines knock as the metallic ringing noise of engine, caused by the auto-ignition of end gas located behind the propagating flame, which, in turn, creates pressure waves in the combustion chamber. This abnormal phenomenon is undesirable because knock can potentially cause severe damage to the piston's head and reduce the efficiency of the engine, as the mixture auto-ignites before reaching the optimum conditions. Hence, fuels used in SI engines are classified by octane ratings, which indicate the propensity of fuels to auto-ignite. The octane rating of a certain fuel is given by the Research Octane Number (RON) and the Motor Octane Number (MON). The RON and MON ratings of a fuel can be obtained from standard test methods in Cooperative Fuel Research (CFR) engine [7,8].

As the demand for fuels with high anti-knock quality is rising, there is a significant interest in blending agents (i.e., octane boosters)

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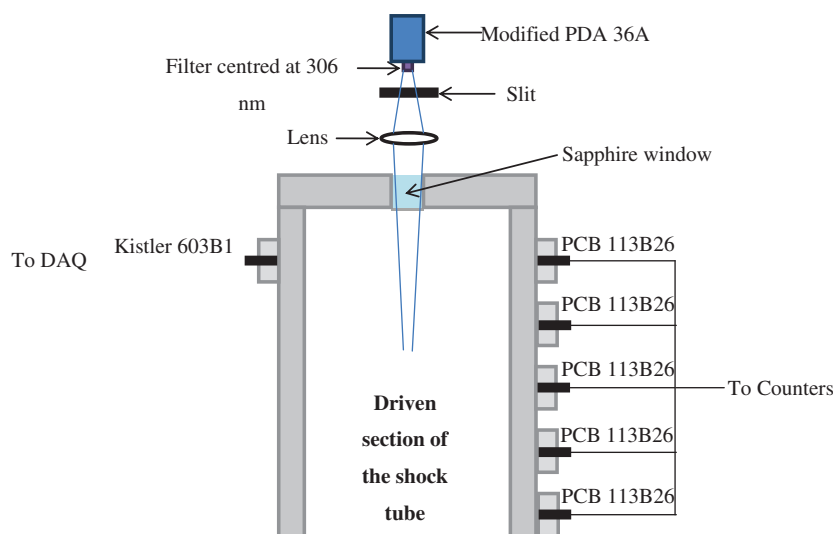


Fig. 1. Experimental setup for ignition delay time measurements.

with conventional gasoline fuels. Alcohols with 1–4 carbon atoms have been proposed for blending with gasoline due to their high octane number [9]. Amongst the alcohols, the butanol isomers offer advantages over ethanol, the most widely used biofuel globally. Firstly, the butanol isomers have a higher energy density than ethanol, resulting in lower volumetric fuel consumption [10]. In addition, unlike ethanol, butanol has a lower tendency to mix with water, which enables higher volume fractions to be blended with gasoline and transport it using existing pipelines [11,12].

There are four butanol isomers: n-butanol, 2-butanol, iso-butanol and tert-butanol. All of the isomers can be produced through biological pathways apart from tert-butanol, which is a petroleum derived product [9,13]. Combustion of the butanol isomers has been studied extensively in shock tubes [14–24]. This greatly contributed to the development of many chemical kinetic models [9,18,22,24–29]. These chemical kinetic models provide a detailed description of the fuel ignition characteristics and hence a better understanding of the fuel/engine interactions through engine-combustion simulations.

The present work focuses on studying the combustion of mixed butanols (MB), a mixture of 68.8% 2-butanol and 31.2% tert-butanol by volume, blended with ternary component gasoline surrogates. The production of combustible mixed butanols from mixed butenes has been patented by the Saudi Aramco [30,31]. The potential use of mixed butanols as oxygenated fuel additives has been studied in DI single cylinder engine by Niass et al. [32], wherein the authors found that MB addition to a commercial RON 97 gasoline resulted in improved knock resistance, higher indicated mean effective pressure (IMEP), and lower particulate emissions. However, no prior effort has been made to investigate mixed butanols combustion at a fundamental level. In this study, a chemical kinetic model has been developed to understand the effects on combustion when adding mixed butanols to gasoline surrogate mixtures. The mechanism is compared against high pressure shock tube ignition delay time measurements for pure mixed butanols and blends of mixed butanols with iso-octane/n-heptane/toluene mixtures.

## 2. Experimental procedure

In this study, ignition delay times were measured using the high-pressure shock tube (HPST) facility at King Abdullah University of Science and Technology (KAUST). The experimental setup has been detailed elsewhere [33] and only brief description is given here. The HPST is made from high purity stainless steel with inner diameter

of 10 cm, driven section of 6.6 m length and driver section can be varied in length (maximum of 6.6 m) depending on the desired test time. The driver and driven sections are separated by a mid-section designed to hold two pre-scored diaphragms. Aluminum diaphragms with various thicknesses and scorings were used depending on the desired pressure behind reflected shock wave ( $P_5$ ). The double diaphragms technique was implemented to achieve a better control of diaphragm rupturing at the desired conditions. Moreover, the facility has two stainless steel mixing vessels attached to the driven section for gaseous air/fuel mixtures preparation. The mixing vessels and the shock tube are vacuumed using turbomolecular pumps to remove impurities. The driven section of the HPST, the mixing vessels and the connecting tubes can be heated to 100 °C to avoid fuel condensation. Five equally separated PCB 113B26 piezoelectric pressure transducers (PZT) are placed axially in the last 1.5 m of the driven section to measure incident shock speed. The pressure time-history of the activity inside the shock tube is recorded using Kistler 603B1 PZT located 1 cm away from the HPST end-wall. OH\* chemiluminescence, light emissions at 306 nm, is monitored using a modified PDA36A detector via Sapphire window in the end-wall. Schematic of the experimental setup in the driven section is shown in Fig. 1.

Gaseous mixtures were prepared by injecting liquid fuel into two evacuated and heated (100 °C) stainless steel mixing vessels. Fuel partial pressure was kept at two-thirds or less of the maximum saturation vapor pressure. Oxygen (purity 99.999%) and nitrogen (purity 99.999%), supplied by Abdullah Hashim Gases, were mixed with the fuel in the mixing vessels to reach desired equivalence ratio. A magnetically driven stirrer was used for at least one hour to mix the fuel vapor with air and produce homogenous mixture. When filling the driven section with air/fuel mixture, butanol has the tendency to adsorb to the shock tube walls. To minimize the adsorption effect, a passivation technique was performed in which the driven section was overfilled by the air/fuel mixture beyond the initial pressure. After that, the excess gas was evacuated from the shock tube until optimal pressure was achieved. The passivation technique is adopted from Stranic et al. [14] shock tube study on butanol isomers. The driver section was pressurized with either pure helium or helium–nitrogen mixture based on the required test time. Refer to [34,35] for further details on the driver gas tailoring technique to extend shock tube test times. The mid-section was filled with the driver gas at half the pressure of the driver section. Then, the shock wave was initiated by venting the middle section, which causes the diaphragms to rupture due to the large pressure gradient between the driver and driven sections.

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