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Ignition and combustion characteristics of 2-methylhexane in a micro flow reactor with a controlled temperature profile

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Abstract: Ignition and combustion characteristics of 2-methylhexane/air mixtures were investigated using a micro flow reactor with a controlled temperature profile. Stable weak flames in the low-velocity region were experimentally observed and computationally simulated using a detailed chemical kinetic model. At atmospheric pressure conditions, distinct two luminous weak flames at intermediate and high temperatures were observed. At higher pressures, another weak flame at the low temperature region was also distinguished. Computational results also showed that there are co-existing three heat-release-rate peaks which agreed the experimental observations. With an increase of pressure, the blue and cool flames were intensified and the hot flame was weakened suggesting that the low and intermediate temperature flames in the three-stage ignition process become more prominent at high pressure conditions. The current experimental and computational results are being investigated further to reveal the underlying chemical mechanisms of 2-methylhexane/air ignition and combustion.

Introduction

The ignition behavior of real petroleum fuels in engines plays an important role in determining power output, efficiency, and emissions. For a detailed understanding of fuel ignition processes, each hydrocarbon molecule should be studied independently and their detailed chemical kinetic models developed. However, this is not possible for real fuels, as they are made up of hundreds of different hydrocarbon molecules. Thus, molecules with similar structures are often grouped together and surrogate fuels are formulated to match important target properties. With the chemical and physical properties of these surrogate fuels similar to those of the real fuel, it becomes easier to develop simpler models that are computationally less expensive [1, 2].

Blends of *n*-heptane and iso-octane, also called primary reference fuels (PRFs) have been used as surrogates to study gasoline in many studies [3,4]. Often researchers add toluene to PRFs (TRFs) to better match the gasoline composition, multi-stage ignition properties, and ignition delay times [5,6]. Mueller et al. [7] proposed a scheme for diesel surrogate formulation by matching target properties. The scheme can be used to formulate gasoline fuel as well. Some of the target gasoline properties to be considered during surrogate formulation are hydrogen to carbon (H/C) ratio, chemical composition, research octane and motor octane numbers (RON, MON), and premixed laminar flame speeds.

In recent studies [8,9], we employ a strategy to formulate multicomponent surrogates with up to 10 components representing real fuels. One possible candidate to represent lightly branched alkanes in real gasoline is 2-methylhexane. To use such a complex surrogate system, it is required to understand detailed ignition and combustion characteristics of each individual component. Thus, the current study focuses on multi-stage ignition characteristics of 2-methylhexane using a micro flow reactor with a controlled temperature profile (MFR).

MFR has been employed to study single stage ignition and multiple ignition phenomena of various fuels [10-18]. Distinctive combustion phenomenon depending upon the inlet fuel/oxidizer mixture flow velocity has been observed. At relatively higher inlet velocities, a stable normal flame was observed. Oscillating flames with rapid extinction and ignition (FREI) were observed at intermediate velocities, while stable weak flames were observed at a very low inlet velocity. The stable weak flames at low inlet velocity correspond to ignition phenomena of the fuel under study [12]. Furthermore, MFR has unique characteristics wherein multi-stage oxidation can be physically observed. Various studies have been conducted to investigate the multi-stage oxidation of different fuels using MFR [11, 14-18]. Thus, a multi-stage oxidation phenomenon that occurs at low inlet velocities in the MFR is the specific focus in this study.

Approach

A typical MFR setup has been employed to study multi-stage oxidation of 2-methylhexane/air mixtures. A Hydrogen flat-flame burner was used to generate the desired temperature profile on the inner wall of the reactor. The wall temperature was measured using a K-type thermocouple inserted into the exit of the reactor. A Nikon digital camera was employed to record flame images. A quartz tube of 1 mm inner diameter (ID) was employed as the reactor, since at higher pressures (e.g. 2 atm and above) the quenching diameter reduces. A larger ID reactor may lead to flame flashback at such elevated pressures. A gaseous mixture of 2-methylhexane and nitrogen (N₂) was prepared and kept in a heated fuel tank (373 K) at pressures of 5.5 atm. The flow of oxygen (O₂) and 2-methylhexane/N₂ into MFR was controlled by calibrated mass flow controllers. The ratio of O₂ and N₂ was kept the same to that of air (i.e., 21% O₂, 79% N₂). The pressure inside the MFR was controlled using a pressure control valve and was varied from 1 atm to 5 atm.

The oxidation of 2-methylhexane/air mixtures was simulated using a detailed chemical kinetic model presented by Sarathy et al. [1]. One-dimensional steady computations were conducting using PREMIX code in CHEMKIN PRO [19]. Computations were done on fixed gas temperature without solving the energy equation. It should be noted that a more accurate method of simulating these experiments is to add the heat convection term between the gas phase and the wall to the energy equation, as performed by [12-18] using non-commercial software. However, in this study a commercial version of CHEMKIN was required to deal with the large size of the 2-methylhexane detailed chemical kinetic model, which cannot be utilized in non-commercial codes. Currently, a CHEMKIN PRO user routine is being built to solve the energy equation, which would account for heat losses between the gas and reactor wall due to convection. All experiments and computations were conducted for stoichiometric fuel/air mixture.

Results and Discussion

Characteristics of weak flame at atmospheric pressure

Stable weak flames with very weak luminescence were observed at the mixture inlet velocity of 2 cm/s. Only two distinctive flames were identified at atmospheric pressure; a hot flame downstream was observed roughly at 1150 K and a broad blue flame relatively upstream. The luminosity of the hot flame was much higher than that of blue flame. This confirms two distinctive reaction zones for oxidation of 2-methylhexane at atmospheric pressure. Three distinctive heat release rate (HRR) peaks were obtained from the computations at 1 atm, as shown in Figure 1. However, the first peak at low temperature was smaller and broader compared to intermediate and high temperature peaks indicating that low temperature heat release

is not very significant at atmospheric pressure. This is supported by the fact that no weak flame was observed at low temperatures in the experiments at similar conditions. This suggests that intermediate and high temperature HHR peaks corresponds to hot and blue flame, which were physically observed. Thus, double stage oxidation phenomenon of 2-methylhexane at atmospheric pressure was confirmed both experimentally and computationally.

Hori et al. studied the dependence of weak flame characteristics on octane number [15]. Comparing the current results of 2-methylhexane (RON = 44) with published n-heptane (RON = 0) and iso-octane (RON = 100), weak flame dependence on octane number were confirmed as claimed by Hori et al. They did not observe any low temperature weak flame for PRF50, which is very close to the fuel used in current study in terms of RON. Moreover, the wall temperatures at the hot flame location for n-heptane was reported to be 1131 K, for 2-methylhexane was found to be 1150K and for iso-octane was 1168 K. This confirms the hot flame position dependence on octane number first observed by Hori et al [15].

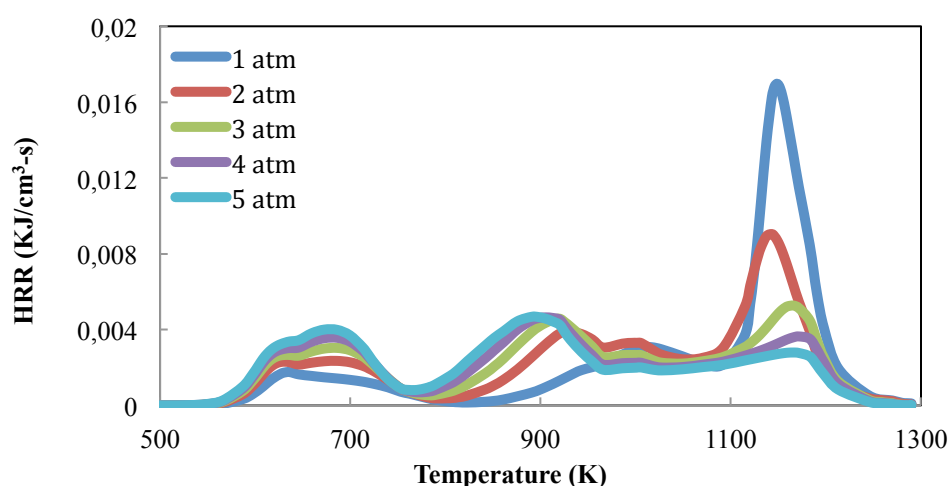


Figure 1. Computed HRR at measured wall temperature.

Characteristics of weak flame at elevated pressures

Figure 2 represents the effect of pressure on the ignition phenomena of 2-methylhexane in the MFR. As the pressure is raised to 2 atm, a weak flame at low temperature appears, denoted as the cool flame. As the pressure is raised further up to 5 atm, the luminosity of the cool flame increases with pressure. At 5 atm, a distinctive three-stage oxidation phenomenon was observed. Furthermore, at higher pressures, the blue flame became stronger and broader while the hot flame became relatively weaker and broader. This suggests an increase in the importance of low and intermediate temperature heat release as the pressure increases. Similar observations were concluded from computational results (Figure 1). The weak and broad HRR peak at low temperature became stronger as the pressure was increased from 1 atm to 5 atm. The high temperature HHR peak, which was strongest at atmospheric pressure, weakened with increasing pressure. Overall, the experimental and computational results and trends qualitatively agreed with each other.

Comparing again with the work of Hori et al. [15], it was observed that the of 2-methylhexane weak flame response to a pressure change had intermediate characteristics to that of n-heptane and iso-octane and were close to that of PRF50.

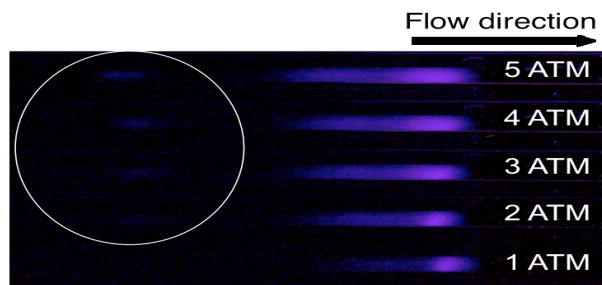


Figure 2. Weak flame images of 2-methylhexane at different pressures.

Conclusions

Multi-stage oxidation and heat release characteristics of 2-methylhexane were studied using a micro flow reactor with a controlled temperature profile. At atmospheric pressure, intermediate and high temperature oxidation was observed. The computed low temperature HHR peak was weak and hence no flame at this region was observed. As the reaction pressure was increased, the importance of low temperature oxidation was observed. A cool flame appeared and the HHR peak at low temperature became significant. Furthermore, the dependence of weak flame characteristics on octane number was confirmed, as weak flame characteristics of 2-methylhexane at atmospheric pressure and elevated pressures lied in between to that of *n*-heptane and iso-octane.

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References

- [1] S.M. Sarathy, C.K. Westbrook, M. Mehl, W.J. Pitz, C. Togbe, P. Dagaut, H. Wang, M.A. Oehlschlaeger, U. Niemann, K. Seshadri, P.S. Veloo, C. Ji, F.N. Egolfopoulos, T. Lu, *Combust. Flame*, 158 (2011) 2338-2357.
- [2] E.J. Silke, H.J. Curran, J.M. Simmie, *Proc. Combust. Inst.*, 30 (2005) 2639-2647.
- [3] H.J. Curran, W.J. Pitz, C.K. Westbrook, C.V. Callahan, F.L. Dryer. *Proc. Combust. Inst.*, 27 (1998), 379-387.
- [4] P.A. Glaude, V. Conraud, R. Fournet, F. Battin-Leclerc, G.M. Côme, G. Schacchi, P. Dagaut, M. Cathonnet, *Energy Fuels*, 16 (2002), 1186-1195.
- [5] W.J. Pitz, N.P. Cernansky, F.L. Dryer, F.N. Egolfopoulos, J.T. Farrell, D.G. Friend, H. Pitsch, SAE 2007-01-0175, 2007
- [6] B.M. Gauthier, D.F. Davidson, R.K. Hanson, *Combust. Flame* 139 (2004) 300-311.
- [7] C.J. Mueller, W.J. Cannella, T.J. Bruno, B. Bunting, H.D. Dettman, J.A. Franz, M.L. Huber, M. Natarajan, W.J. Pitz, M.A. Ratcliff, K. Wright, *Energy Fuels*, 26 (2012) 3284-3303.
- [8] S.M. Sarathy, G. Kukkadapu, M. Mehl, W. Wang, T. Javed, S. Park, A. Elwardani, A. Farooq, M.A. Oehlschlaeger, A. Farooq, W.J. Pitz, C-J. Sung, *Proc. Combust. Inst.*, Accepted 2014.
- [9] M. Mehl, J.Y. Chen, W.J. Pitz, S.M. Sarathy, C.K. Westbrook, *Energy Fuel*, 2011, 25, 5215-5223.
- [10] K. Maruta, T. Kataoka, N.I. Kim, S. Minaev, R. Fursenko, *Proc. Combust. Inst.*, 30 (2005) 2429-2436.
- [11] A. Yamamoto, H. Oshibe, H. Nakamura, T. Tezuka, S. Hasegawa, K. Maruta, *Proc. Combust. Inst.*, 33 (2011) 3259-3266.
- [12] Y. Tsuboi, T. Yokomori, K. Maruta, *Proc. Combust. Inst.*, 32 (2009) 3075-3081.
- [13] T. Kamada, H. Nakamura, T. Tezuka, S. Hasegawa, K. Maruta, *Combust. Flame*, 161 (2014) 37-48.
- [14] S. Suzuki, M. Hori, H. Nakamura, T. Tezuka, S. Hasegawa, K. Maruta, *Proc. Combust. Inst.*, 34 (2013) 3411-3417.
- [15] H. Oshibe, H. Nakamura, T. Tezuka, S. Hasegawa, K. Maruta, *Combust. Flame*, 157 (2010) 1572-1580.
- [16] H. Nakamura, A. Yamamoto, M. Hori, T. Tezuka, S. Hasegawa, K. Maruta, *Proc. Combust. Inst.*, 34 (2013) 3435-3443.
- [17] M. Hori, A. Yamamoto, H. Nakamura, T. Tezuka, S. Hasegawa, K. Maruta, *Combust. Flame*, 159 (2012) 959-967.
- [18] M. Hori, H. Nakamura, T. Tezuka, S. Hasegawa, K. Maruta, *Proc. Combust. Inst.*, 34 (2013) 3419-3426.
- [19] CHEMKIN PRO 15112, Reaction Design, 2013.