Numerical Study of Radical Reaction in Kerosene Auto-ignition

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Abstract. Spontaneous emission signal had different curves of kerosene's auto-ignition in shock tube under different temperature conditions, and OH^* radicals concentration time history was numerically investigated. Two component surrogate fuel model (n-decane+trimethylbenzene) was used to validate consistency of its ignition delay time data with kerosene. Then simulation of OH^* time history during reaction was carried out using the surrogate fuel model's combustion mechanism. OH^* radicals' sensitivity analysis and reaction paths of production and consumption were investigated under different temperatures. The results show that the difference of dominant reactions for radicals' consumption lead to different curves of OH^* radicals traces, which was that two peaks curve would present more easily under lower temperature and one peak curve under higher temperature.

Introduction

Aviation kerosene is a complex fuel containing naphthenic hydrocarbon, alkane and aromatic hydrocarbon. Its fundamental combustion characteristics are important for engine's design modification, combustion efficiency improvement, and el al. Many research group has conducted ignition delay time measurements on the shock tube system. Our lab has set up an aerosol shock tube system, and carried out ignition delay time study of several different hydrocarbon fuels. Ignition time after the reflected shock wave was the key parameter of judgement, and there are two ways. One way is the rise step of pressure curve after combustion, and the other is radicals' emission during combustion[1]. Optical emission is more prior to adopt. Emission signal of CH* or OH* collected by PMT (431nm or 306nm nearby) was used as the initiation time of ignition[2]. According to the premixed fuel with mass diluent gas, ignition delay time differences between side wall or end face measurement can be ignored[3]. We have studied the ignition delay time of RP-3 under different temperatures and equivalence ratios, and accumulated plenty of time data. We observed the two peaks curve in OH^* emission signal ,which is more obvious in low temperature. This phenomena was coincident with the absorption spectrum measurement results[4].

In order to analysis OH* production process from kinetic field, the reaction process should be studied according to combustion mechanism. For kerosene's complex constituents, suitable surrogate fuel model was always adopted. The surrogate fuel model has been widely studies both in China and aboard, which included single component, three components and six components model[5-7].Honnet, et al[9] from Aachen University developed a two components model (80% n-decane+20%trimethylbenzene) and validated the mechanism through shock tube, rapid compression machine, and premix combustion experiments.

The simulation results with Honnet's mechanism was close to our RP-3 kerosene (equivalence formular:$C_{10}H_{22}$) ignition delay time data, as shown in Fig.1. So this article investigated OH* radicals production process and reaction paths based on Honnet's mechanism using CHEMKIN-PRO.

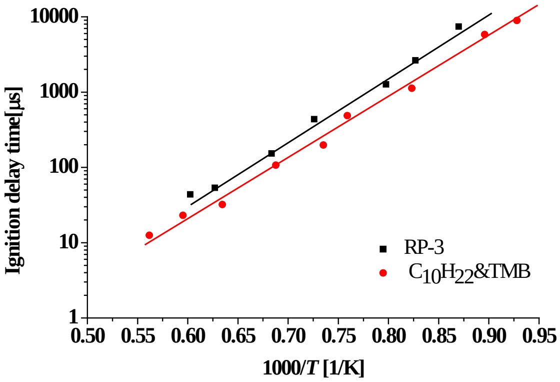
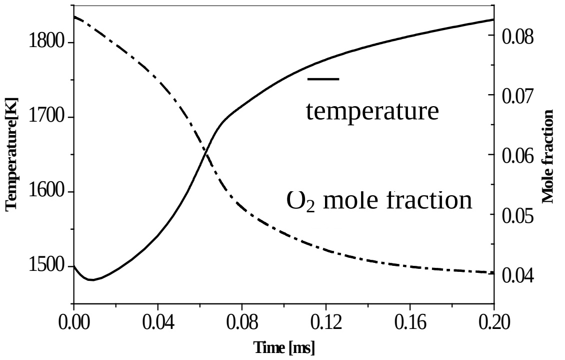


Fig.1 Comparison of ignition delay times of kerosene and surrogate fuel[10]

Combustion mechanism and validation

The mechanism contains 119 species and 527 reactions, whose main cracking reactions can be searched from Ref[9]. Ignition process was simulated under T=1500K, P=1atm, and equivalence ratio=1.0, the temperature and O_2 mole fraction were show in Fig.2.



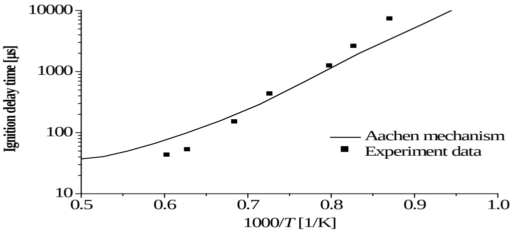


Fig.2 Temperature and O_2 mole fraction curve(T=1500K,P=1atm,ϕ=1.0)

Fig.3 Comparison of ignition delay time data of experiments and simulation (P=1atm,ϕ=1.0)

It can be concluded that O_2 mole fraction begin to decrease from beginning, and temperature decrease at the first 0.01ms and then increase, which due to radicals accumulation at the initiation stage and endothermic reaction. The ignition delay time data and simulation results were compared under broader temperature range and shown in Fig.3. The data coincide with each other mainly in intermediate temperature range (about 1200~1500K).

OH radicals sensitivity analysis and reaction path analysis

OH* radicals, remarking ignition delay time, was used to conduct sensitivity analysis (Fig.4). Elementary reactions, R1,R3,R30,R46,R50,R67,R69,R107,R112,R138, were all in favour of ignition delay time decreasing, in which R1 had highest sensitivity. While R8,R34,R72 were all in favour of increasing, and R34 had highest sensitivity.

Table 1. Main reactions influencing ignition delay time（T=1700K，P=1atm，ϕ=1.0）

Elementary reaction number	Reaction formula	Effect on ignition delay time	Elementary reaction number	Reaction formula	Effect on ignition delay time
R1	$H+O_2$<=>OH+O	（reduce）	R67	$OH+CH_3$<=>$PXCH_2+H_2O$	（reduce）
R3	$OH+H_2$<=>H_2O+H	（reduce）	R69	CH_3+HO_2<=>CH_3O+OH	（reduce）
R8	HO_2+OH<=>H_2O+O_2	（increase）	R72	CH_3+H(+M)<=>CH_4(+M)	（increase）
R30	HCO+M<=>CO+H+M	（reduce）	R107	C_2H_2+O<=>HCCO+H	（reduce）
R34	HCO+OH<=>CO+H_2O	（increase）	R112	C_2H_3(+M)<=>C_2H_2+H(+M)	（reduce）
R46	$TXCH_2+O_2$ =>CO+OH+H	（reduce）	R138	C_2H_4+OH<=>C_2H_3+H2O	（reduce）
R50	$PXCH_2+O_2$ =>CO+OH+H	（reduce）			

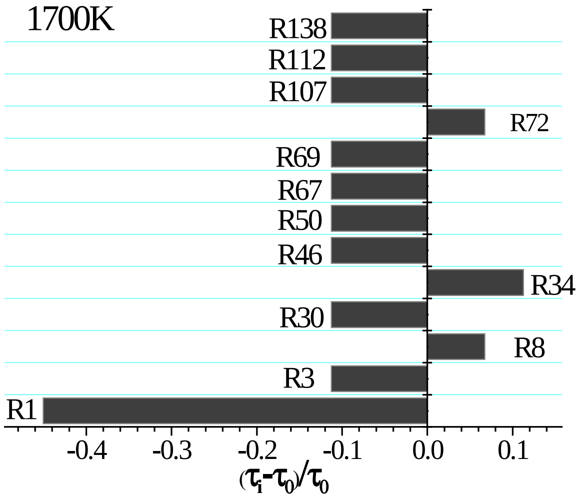
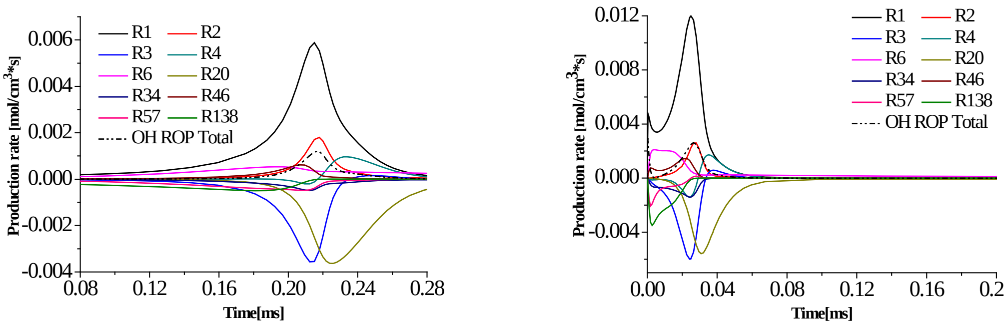


Fig.4 Sensitivity analysis of ignition delay time (T=1700K, P=1atm, ϕ=1.0)

Fig.5 compared OH^* reaction paths under different temperatures. OH^* production was due to R1, but reaction rate were different under ignition temperature of 1400K and 1700K. OH^* production from reaction R1 increased gradually in lower temperature and reached peak in 0.22ms. While in higher temperature, OH^* reached peak in a short time for R1, fell back in a small range and reached peak again in 0.03ms. For OH^*'s consumption, reactions R3 and R20 dominated and reached consumption peak slightly before R1's production peak under lower temperature. For mass consumption before production peak, OH^* emission curve exhibited double peaks. When temperature was higher, OH^* radicals were consumed from beginning until the production peak, so the global consumption lead to one peak structure of OH^* emission curve.



（a）1400K　　（b）1700K

Fig.5 OH radical reaction path analysis under different temperatures（P=1atm，ϕ=1.0）

Conclusion

Surrogate fuel model (n-decane+trimethylbenzene) mechanism was used to numerical study the OH* radicals reaction process of RP-3 kerosene's auto-ignition in shock tube, and dominant production and consumption reactions were find out. Double peaks curve of OH^* emission was found to be caused by different leading production and consumption reaction paths after comparing reaction paths under different temperatures. Different time scale of production peak and consumption peak lead double peaks under lower temperature. While more consumption reaction paths caused higher global consumption under higher temperature and thus one peak curve of OH^* emission.

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