

Experimental and kinetic investigation of n-decane/1,3,5-trimethylbenzene oxidation

Zhen-Yu Tian^{1,2,*} and Bing-Yin Wang^{1,2}

¹ Institute of Engineering Thermophysics, Chinese Academy of Sciences, Beijing, China

² University of Chinese Academy of Sciences, Beijing, China

* Corresponding author: tianzhenyu@iet.cn

To better enhance the combustion efficiency and reduce the pollutant emissions, it is necessary to develop a detailed kinetic model describing the combustion characteristics of kerosene. Since kerosene are composed of hundreds of chemical components which makes the model establishment impossible, it has been widely accepted by the researchers to use representatives to emulate the parent fuel and reduce the size of models. Among the surrogates, one of the simplest is the one consisting of 80% n-decane and 20% 1,3,5-trimethylbenzene (TMB135) by mass with the H/C ratio (2.0) close to that of 1.92 for gas turbine fuel JP-8. Although some previous studies relevant to the combustion of surrogate and TMB135 in shock tube, laminar and counter-flow flames are available, there still remains a lack of studies on the low-temperature oxidation of such combination in micro-kinetic perspective regarding the speciation analysis, particularly in the negative temperature coefficient (NTC) region at atmospheric pressure under rich conditions.

In this work, the low temperature oxidation of neat TMB135 and n-decane/ TMB135 mixture as a surrogate was investigated in a jet-stirred reactor at 500-1100 K. In the experiments, 1.0% vaporized neat TMB135 or n-decane/TMB135 surrogate (77%/23% by mole ratio) mixture with 6.0% or 7.2% O₂, respectively, corresponding to $\Phi = 2.0$, were introduced into the reactor at a constant flow rate of 1000.00 standard cubic centimeter per minute (sccm). Reaction products were sampled and analysed using online GC equipped with TCD and FID. The estimated uncertainty was about $\pm 5\%$ for major species and $\pm 10\%$ for intermediates. Based on the experimental observations and previously proposed models of TMB135 by Di éart et al. [1] and n-decane by Herbinet et al. [2], a combined kinetic model was used for ROP and sensitivity analysis.

For the n-decane/ TMB135 mixture, the major species and intermediates exhibited general NTC behavior in 550-800 K. The n-decane addition is observed to result in less formation of aromatics with lower peak concentrations at low temperatures compared to that in neat TMB135. The flux analysis indicate that TMB135 in the surrogate is mainly consumed by the H-abstractions by OH radical in the NTC region, while neat TMB135 is mainly consumed by the H-abstractions by H-atom, OH and CH₃ radicals at relatively high temperature (see Fig. 1). The H-abstraction in the side methyl groups of TMB135 by OH radical has the most significant promoting effect for TMB135 in surrogate oxidation in the NTC region, while this reaction plays a strong inhibiting effect in the neat TMB135 oxidation.

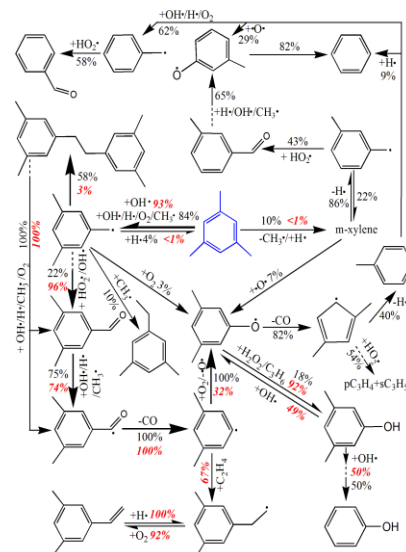


Fig. 1 ROP analysis

References

- (1) Di éart, P.; Kim, H.H.; Won, S.H.; Ju, Y.; Dryer, F.L.; Dooley, S.; Wang, W.; Oehlschlaeger, M.A. *Fuel* **2013**, 109 125-136.
- (2) Herbinet, O.; Husson, B.; Ferrari, M.; Glaude, P.A.; Battin-Leclerc, F. *Proc. Combust. Inst.* **2013**, 34: 297-305.