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Zhandong Wang

Experimental and Kinetic Modeling Study of Cyclohexane and Its Mono-alkylated Derivatives Combustion

Doctoral Thesis accepted by
the University of Science and Technology of China,
Hefei, China

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Supervisor's Foreword

The combustion of fossil fuels provides most of the energy used worldwide, and it promotes the growth of society and the economy. However, large amounts of emitted pollutants are harmful to human health and to the sustainability of human civilization. The design of high-efficiency low-emission engines and the development of detailed kinetic models of fossil fuels are crucial to alleviating the energy shortage and reducing pollution. Cycloalkanes are an important component of fossil fuels and their surrogates. In China, for example, No. 3 Kerosene has large mass fraction of cycloalkanes, and the recent discovery of oil sands may contain larger fractions of cycloalkanes. The combustion of cyclohexane and its derivatives produces large amounts of dienes (carcinogenic 1,3-butadiene) and cyclic intermediates, and it has a relatively high sooting tendency.

The object of this Ph.D. thesis is to clarify the combustion chemistry of cyclohexane and its two mono-alkylated derivatives (methylcyclohexane and ethylcyclohexane), which are commonly chosen as surrogate components for transport fuels. The pyrolysis and laminar premixed flames of these three model compounds were studied using state-of-the-art synchrotron radiation photoionization mass spectrometry. Their initial reaction pathways during combustion were calculated with high-level quantum chemistry methods, and the rate constants were evaluated. A detailed kinetic model was developed and validated against experimental data covering a wide range of combustion conditions, including pyrolysis at various pressures, flame structure at low pressures, as well as species concentrations from jet-stirred reactor oxidation at intermediate and high temperatures, ignition delay times, and laminar flame speeds. This model contributes to understanding the combustion chemistry of these cycloalkanes (initial decomposition pathways, distribution of intermediates, and formation of air pollutants), developing combustion models for substituted cycloalkanes with long alkyl side chains and/or multiple side chains, and it has application to engine and fuel design, and emission control.

Hefei, People's Republic of China
September 2017

Prof. Fei Qi

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Z. Wang, L. Ye, W. Yuan, L. Zhang, Y. Wang, Z. Cheng, F. Zhang, F. Qi, *Combust. Flame* 161 (2014) 84–100.

Z. Wang, H. Bian, Y. Wang, L. Zhang, Y. Li, F. Zhang, F. Qi, Proc. Combust. Inst. 35 (2015) 367–375.

Z. Wang, L. Zhao, Y. Wang, H. Bian, L. Zhang, F. Zhang, Y. Li, S.M. Sarathy, F. Qi, *Combust. Flame* 162 (2015) 2873–2892.

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