

乙醇均质压燃燃烧的化学反应动力学模拟

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摘要 应用0-D单区模型耦合乙醇氧化反应详细化学动力学机理, 对乙醇均质压燃燃烧反应化学动力学进行了数值模拟研究。分析了乙醇氧化消耗的主要途径及乙醇的燃烧反应机理中的关键中间产物和重要的基元反应, 并总结了乙醇总体氧化流程。研究表明: 在乙醇氧化消耗的主要途径中, $C_2H_5OH+OH \rightarrow$ 产物占主导, 单个基元反应中以R145 $C_2H_5OH+OH=CH_3CH_2O+H_2O$ 为主, 其次为R144 $C_2H_5OH+OH=CH_3CHOH+H_2O$ 。乙醇氧化经裂解反应、脱氢反应最终形成支链反应, 乙氧基 C_2H_5O 的三种同分异构体在链分支中决定了链分支的进行方向。

关键词 [动力机械及工程](#) [均质压燃](#) [乙醇](#) [模拟计算](#) [化学动力学](#)

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Numerical simulation on chemical reaction kinetics of ethanol HCCI combustion

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Abstract The numerical simulation was performed on the homogeneous charge compression ignition(HCCI) combustion of ethanol by means of the 0-D single zone model coupled with the modified detailed chemical kinetics mechanism of ethanol oxidation reaction. The main consuming paths of ethanol oxidation as well as the key intermediate products and the important elementary reactions in the ethanol combustion reactions were sorted. The results show that the reaction path $C_2H_5OH+OH \rightarrow$ products is a dominant path over all key ethanol consuming paths, and the ethanol oxidation reaction R145: $C_2H_5OH+OH=CH_3CH_2O+H_2O$ is the most important elementary reaction and the reaction R144: $C_2H_5OH+OH=CH_3CHOH+H_2O$ is the second important in all important elementary reactions. The unimolecular decomposition and dehydrogenation of ethanol initiate the branched chain reaction, and the 3 isomers of radical C_2H_5O determine the direction of the reaction chain branching.

Key words [power machinery and engineering](#) [HCCI](#) [ethanol](#) [numerical simulation](#) [chemical reaction kinetics](#)

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