Theoretical Investigation of the Butanol Combustion Mechanism

Gladson de Souza Machado (PG), Glauco F. Bauerfeldt (PQ)

Departamento de Química, Instituto de Ciências Exatas, UFRuralRJ

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INTRODUCTION

Attempts to avoid the dependence on fossil fuels and the search for sustainable and renewable energy sources are issues of great importance worldwide[1]. An alternative fuel is butanol and, despite the apparent advantages over other biofuels, as ethanol, a systematic study of the combustion profile is needed. Hence, the main goal of this work is the investigation of the most important reactions in butanol combustion mechanism.

METHODS

The kinetic model proposed by Sarathy et al.,[2] modified to include the NOx chemistry has been adopted to simulate the combustion of butanol. The coupled ordinary differential equations have been integrated using the numerical method DVODE available in the Kintecus ® software.[3] Rate Analysis (RA) and Sensitivity Analysis (SA) have been performed in order to identify the most important reactions to the initiation of the mechanism and to the ignition. The simulation has been done at 1332 K and 1.73 atm, with equivalence ratio one, four percent of oxygen in the mixture, using argon as bath gas and assuming constant volume, in order to reach the experimental shock tube conditions.

RESULTS AND DISCUSSION

The chemical kinetic model for the combustion of butanol is originally composed by 2335 reactions and 426 species. In this mechanism, 65 reactions are responsible for the consumption of butanol.

RA suggests that, at 1332 K, butanol is consumed, in the beginning of the reaction (at a time value corresponding to 0.5% of the ignition delay time), mostly by C-C bond cleavage and dehydration reactions (which sum up to 40.0% of the flux of butanol consumption). Other important channels are the hydrogen abstraction reactions by hydrogen atoms (28.5%) and hydroxyl radicals (28.5%). At a time value corresponding to 2% of the ignition delay, this ranking is changed and hydrogen abstraction by hydrogen atoms is found as the most relevant (34.0%). Among O_2 reactions, $O_2+CH_2OH \rightarrow CH_2O+HO_2$ is suggested to be the most important, followed by $H+O_2 \rightarrow O+OH$. It is important to notice that the CH_2OH is the main product of the unimolecular C-C bond dissociation. Similar analysis for other simulations performed at different initial conditions was done.

SA confirm that the C-C cleavage and dehydration reactions are the most important for the butanol consumption, but at the ignition delay time the reaction butanol is mostly removed by OH radicals, which arise from the $H+O_2 \rightarrow O+OH$ reactions. The sensitivity coefficient for this reaction is high, also being the most important for the formation of oxygen atoms and for the raise of the temperature.

CONCLUSIONS

Our results suggest that the unimolecular reactions of butanol play a fundamental role in the initiation of the combustion. Moreover, the $H+O_2 \rightarrow O+OH$ reaction was shown to be highly important in the ignition delay time. Hydrogen abstraction reactions showed the highest contributions to the rate of consumption of butanol at the ignition delay time.

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