

**EXPERIMENTAL AND KINETIC MODELING STUDY OF THE AUTO-
IGNITION CHARACTERISTICS OF THE FOUR ISOMERS OF BUTANOL**

By

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ABSTRACT

The autoignition characteristics of the four isomers of butanol (1-butanol, 2-butanol, iso-butanol, and tert-butanol) have been experimentally studied in a shock tube at high temperatures. Ignition delay measurements were made behind reflected shockwaves for varying butanol/oxygen/argon ratios at temperatures between 1200 and 1800 K and at pressures from 1-4 bar. Emission from electronically excited OH molecules in addition to pressure measurements were used to determine ignition delay. The influence of temperature, pressure, and mixture composition on ignition delay time has been characterized for each isomer. Comparisons were made to a detailed kinetic mechanism developed by the Battin-Leclerc research group at Nancy Université in France in order to validate ignition delay predictions of the mechanism and develop an understanding of the importance of various elementary reactions. Reaction flux and sensitivity analyses show the relative importance of the three competing consumption reactions used in the mechanism: dehydration, unimolecular decomposition, and H-atom abstraction. The consumption of 1-butanol and iso-butanol occurs predominately via H-atom abstraction. The result of this is the formation of alkyl radicals that decompose readily to create a large population of highly reactive H atoms and OH radicals. Dehydration dominates the consumption of the less reactive isomers, 2-butanol and tert-butanol, resulting in the formation of alkene molecules which have a low reactivity.