Revisiting the Kinetics and Thermodynamics of the Low-Temperature Oxidation Pathways of Alkanes: A Case Study using the Pentane Isomers

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1. Introduction
Alkanes are the simplest type of hydrocarbon, so knowledge of the combustion of these compounds is essential to the fundamental understanding of the combustion of all hydrocarbons and oxygenated fuels (e.g., alcohols, large methyl esters, etc.). The low-temperature oxidation of alkanes is of practical importance to the advancement of technologies such as homogeneous-charge compression-ignition (HCCI), premixed-charge compression-ignition (PCCI), and reactivity-controlled compression-ignition (RCCI) engines. Construction of detailed mechanisms describing low-temperature oxidation can be difficult due to the large number of chemical species and reactions involved. Group additivity¹ and rate rule²,³ methods are convenient solutions to this problem. In this study we discuss the implementation of both methods, and improved values used therein, for current and future development of detailed chemical kinetic models.

2. Conclusions
There have been significant changes to the thermochemical properties values and rate coefficients for the species and reactions important to low-temperature oxidation, respectively. By using the most up-to-date thermochemistry group values and rate coefficients from several recent publications, the current model shows very good agreement with experimental data. We show that revisions to both the thermochemistry and the kinetics are required in order to replicate experiments well.

With major updates to thermochemical properties values and recommended rate rules, along with solutions to the long-standing discrepancies in the mechanisms of the PRFs, future work would entail applying the updated thermochemistry values, rate rules, and pathways used in this work to larger straight- and branched-chained alkanes. The oxidation of biofuels should also be reconsidered in light of our results.

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4. References