

KINETIC MECHANISM OF *n*-PENTANE OXIDATION
AND COMBUSTION

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Detailed reaction mechanisms of hydrocarbon oxidation contain hundreds species and thousands reactions and incorporate multiple intermediate molecules, isomers, and radicals. Despite many fundamental advantages inherent in such mechanisms, their use in applied studies of combustion and explosion dynamics is impossible nowadays due to their complexity. In addition, these mechanisms cannot be considered as comprehensive as their applicability is usually limited by certain constraints. This paper continues authors' previous attempts to use an automated algorithm for developing an optimal rather than "maximal" reaction mechanism aimed at correct description of main elementary processes governing the overall reaction rate and formation of principal intermediate and final products. Such a mechanism has a status of nonempirical detailed reaction mechanism as its elementary reactions are fundamentally substantiated. The mechanism has two specific features: (*i*) it does not include reactions of double oxygen attachment (first to a peroxide radical and then to its isomer), i.e., the first attachment is assumed sufficient; and (*ii*) reactions with isomer compounds and their derivatives are not considered because the corresponding oxidation routes are slower than the routes via molecules and radicals of normal structure. The use of the algorithm allows the development of relatively compact oxidation mechanisms for heavy *n*-alkanes. In this paper, such a mechanism has been developed and validated for *n*-pentane. The distinctive feature of the mechanism is that it provides satisfactory description of low-temperature *n*-pentane oxidation with cool and blue flames.