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Detonation Initiation by a Temperature Gradient for a Detailed Chemical Reaction Models MICHAEL LIBERMAN, Uppsala University, ALEXEY KIVERIN, Joint Institute for High Temperatures, Russian Academy of Science, Moscow, Russia, ALEXANDER CHUKALOVSKY, Moscow State University, Moscow, 119991 Russia, MIKHAIL IVANOV, Joint Institute for High Temperatures, Russian Academy of Science, Moscow, Russia — The evolution from a temperature gradient to a detonation is investigated using high resolution numerical simulations for combustion mixture whose chemistry is governed by a detailed chemical kinetics. We employ a model representing an initial linear temperature gradient in the fuel. Emphasis is on comparing the results with previous studies that used simple one-step kinetics. It is shown that the evolution to detonation from temperature nonuniformities is considerably different for one-step kinetics models than for chain-branching kinetic models and it is different in different fuels for the same initial conditions. A detailed chemical model has a profound effect on the validity of Zel'dovich's spontaneous wave concept for detonation initiation by a gradient of reactivity. The evolution to detonation from a temperature gradient is considered for hydrogen-air and methane–air mixtures at different initial pressures. The analysis shows that for a detailed chemical kinetics the temperature gradients, which was thought to appear in the form of hot spots and the like, are not satisfy the criteria to initiate detonation, and the gradient mechanism can not be origin of the deflagration-to-detonation transition.

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