Explicit analytic prediction for hydrogen-oxygen ignition time at temperatures below crossover.

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Abstract

This study addresses ignition of hydrogen-oxygen mixtures when the initial conditions of temperature and pressure place the system below the crossover temperature associated with the second explosion limit. The analysis begins by identifying the minimum set of elementary steps required to describe the ignition history. The resulting short mechanism of eight reactions is further simplified by noting that all chemical intermediates except HO\textsubscript{2} can be assumed to be in steady state during most of the ignition process. A further simplification is obtained by assuming HO\textsubscript{2} to be also in steady state, a very good approximation at atmospheric pressure, yielding the two global steps 2H\textsubscript{2} + O\textsubscript{2} → 2H\textsubscript{2}O and 2H\textsubscript{2}O → H\textsubscript{2}O\textsubscript{2} + H\textsubscript{2}. The numerical integrations indicate that, after a short initiation period, ignition occurs as a thermal runaway that can be described by activation energy asymptotics, yielding an explicit expression that predicts accurately the ignition time for different conditions of initial temperature and composition and atmospheric and moderately large pressures.