

**KINETIC MODELING OF HYDROCARBON  
AUTO-IGNITION FOR CONDITIONS  
RELEVANT TO PULSE DETONATION  
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The operability of Pulsed Detonation Engines (PDE) is considerably dependent on the fuel used. Of particular importance is the fuel reactivity within a wide range of operating conditions covering both regular modes (cold start, repetitive detonation initiation and propagation, cyclic mixture stratification and preheating by hot walls, etc.) and irregular phenomena (initiation failure, pre-ignition, deviation in fuel/air/spark or pre-detonator timing, etc.). Thus, the performance analysis of PDE implies the knowledge of kinetic mechanisms of fuel oxidation.

Currently, heavy liquid hydrocarbon fuels are considered as prospective candidates for practical applications due to their advantages compared to light gaseous compounds. The oxidation mechanisms of heavy hydrocarbon fuels account for thousands elementary reactions and are not suitable for multi-dimensional unsteady performance simulations of various PDE design configurations. Continuing studies of [1–3], this paper presents a semi-empirical oxidation mechanism of a heavy hydrocarbon fuel characterized by the octane number,  $n$ . The fuel is assumed to be a blend of  $(100 - n)\%$   $n$ -heptane and  $n\%$  *iso*-octane. Compared to [1–3], the reaction mechanism was extended to allow computations at low initial pressure and to complete mixture burnout.

Verification of the reaction mechanism has been done by comparing predicted auto-ignition delay times with available data obtained by means of rapid compression machines and shock tube techniques. The experimental conditions close to those attained prior and after shock compression of the reactive mixture in PDE, namely, temperature  $650 \text{ K} < T < 1200 \text{ K}$ , pressure  $1 \text{ bar} < p < 100 \text{ bar}$ , equivalence ratio  $0.5 < \Phi < 2.0$ , were examined. Reduced reaction mechanisms were

also developed which approximate with a good accuracy the results of detailed calculations within ignition delay time. The reduced mechanisms are intended to be applied in the multi-dimensional simulation of processes in PDE.

### References

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