Dynamics of OH*, CH* and CO_2* chemiluminescence in methane and n-hexane mixtures

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Chemiluminescence, which corresponds to the light emitted by excited species as they relax to the ground state, can be found in many combustion processes and is widely used as a marker of heat release rate in flame. OH*, CH* and C_2* radicals and the molecule CO_2* are among those commonly studied. The chemical kinetics of OH* is the most well understood. However, a number of studies have shown that usually admitted proportional relationship between OH* chemiluminescence and heat release rate can be more complex. Furthermore, chemiluminescence of markers with broad emission spectrum, as CO_2* molecule, that is difficult to isolate from background emissions of other species, is even more challenging to correlate with heat release rate.

In order to study this correlation, experiments with methane (T_5 = 1500-2500, Φ = 0.67, 1 and 2, X_{AR} = 0.96) and hexane (T_5 = 1300-1600, Φ = 0.5, 1 and 2, X_{AR} = 0.96) have been conducted behind the reflected shock waves in the Caltech Shock Tube. The tube is composed of three parts separated by two diaphragms and is made of stainless steel. The test section is 2.44-m-long, 7.62 cm in diameter. The test section of the shock tube was equipped with diagnostic instruments located close to the end wall: twelve piezoelectric pressure transducers and two quartz optical windows mounted at 13 mm from the tube end, connected to two solarization-resistant multimode optical fibers with a core diameter of 200 μm. The optical fibers are linked to photomultipliers (Hamamatsu and Thorlabs) equipped with band-pass filters of 306 $\pm$ 5 nm, 410 $\pm$ 5 nm and 430 $\pm$ 5 nm, for detecting the ($A^2\Sigma^+ - X^2\Pi$), ($A^1B^2 - X^1\Sigma^+$) and ($A^2\Delta - X^2\Pi$) transitions of OH*, CO_2* and CH*, respectively.

Experimental data were compared with the detailed reaction model of Mével for methane and Dagaut model for hexane, giving mean errors between 11-26% and 11-28%, respectively. The correlation between OH*, CH* and CO_2* and energy release was found to have a complex dependence on both species and temperature. The emission from the CO2* molecule was found to give the least satisfying result as an ignition marker.

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