

EXPERIMENTAL STUDY OF THE EFFECT OF NO AND NO₂ ON THE OXIDATION OF A MIXTURE OF PRIMARY REFERENCE FUELS

G. Dayma², P. Dagaut¹

¹ICARE-CNRS, 1c avenue de la Recherche Scientifique, 45071 Orléans

²ICARE-CNRS, University of Orléans, 1c avenue de la Recherche Scientifique, 45071 Orléans

BACKGROUND-AIM

Traces of nitric oxides (NO or NO₂) are now well known to promote the ignition of simple fuels. This promoting effect is important in several practical systems among which: (i) the NO-NO₂ conversion by hydrocarbons in recent NO_x-reduction strategies, (ii) the modeling of combustion with exhaust-gas recirculation (EGR) such as in Diesel and Homogeneous Charge Compression Ignition (HCCI) engines and mild combustion. The complex interaction of nitric oxides and fuel mixtures is less understood, especially at high level of NO_x.

METHODS

New experimental results were obtained for the oxidation of primary reference fuels sensitized by NO or NO₂. A mixture of 85% iso-octane and 15% n-heptane (PRF85) has been studied experimentally in a fused-silica jet-stirred reactor at 10 atm and a constant residence time of 0.5 s, over the temperature range 500-1000 K, and for equivalence ratios of 0.2, 0.5 and 0.7. At $\phi = 0.2$, the effect of three initial mole fractions of NO were studied (XNO = 0, 50, and 200 ppm) as well as two initial mole fractions of NO₂ (XNO₂ = 0 and 50 ppm). At $\phi = 0.5$ and 0.7, XNO = 200 ppm was used in order to investigate the influence of the equivalence ratio. Finally, at $\phi = 0.2$, two temperatures were selected (T = 660 K, the maximum of the cool flame, and T = 750 K, the maximum of the negative temperature coefficient, NTC) and the initial mole fraction of NO was varied (XNO = 0, 25, 50, 75, 100, 125, 150, 175, 200, 250, 300, 500, 1000, and 2000 ppm). Concentration profiles of reactants, stable intermediates, and final products have been obtained by sonic probe sampling followed by on-line and off-line GC-FID/TCD and FTIR analyses.

RESULTS

The sensitized oxidation of this PRF85 under these conditions showed the three regimes of oxidation well-known for large hydrocarbons, namely cool flame, NTC, and high temperature oxidation. Both NO and NO₂ show a strong effect on the low and intermediate temperature ranges. Results show that NO and NO₂ have similar effects because, since the lowest temperatures, NO is quickly converted into NO₂. When XNO increases, the intensity of the cool flame decreases while the reactivity in the NTC increases. At $\phi = 0.2$, and for XNO = 200 ppm, the NTC has completely disappeared whereas the cool flame disappears for an NO initial mole fraction between 300 and 500 ppm.

CONCLUSIONS

In this experimental work, nitric oxides were shown to have huge impact on the reactivity of a PRF85 over a wide range of temperature. A detailed kinetic mechanism, including low- and high-temperature for iso-octane and n-heptane, will be required in order to understand the complex interactions between NO_x and these two hydrocarbons.

ACKNOWLEDGEMENTS

Support from the CAPRYSESSES project (ANR- 11-LABX-006-01) funded by ANR through the PIA (Programme d'Investissement d'Avenir) is gratefully acknowledged.