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▶ To cite this version:

Nicolas Villenave, Guillaume Dayma, Pierre Brequigny, Fabrice Foucher. Experimental investigation of NOx impact on ignition delay times for lean H2 /Air mixtures using a rapid compression machine under ice conditions. 5th International RCM Workshop, Jul 2024, Milan, Italy. hal-04906713

HAL Id: hal-04906713 https://hal.science/hal-04906713v1

Submitted on 22 Jan 2025 $\,$

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EXPERIMENTAL INVESTIGATION OF NO_x IMPACT ON IGNITION DELAY TIMES FOR LEAN H_2/AIR MIXTURES USING A RAPID COMPRESSION MACHINE UNDER ICE CONDITIONS

N. Villenave¹, G. Dayma^{2,3}, P. Brequigny¹, Fabrice Foucher¹ ¹Univ. Orléans, INSA-CVL, PRISME, EA 4229, F45072, Orléans, France ²CNRS ICARE, Avenue de la Recherche Scientifique, 45071 Orléans Cedex 2, France ³Université d'Orléans, Orléans, Cedex 2, France

Introduction

- \Box The transport sector is the second most polluting sector: CO₂ emissions = 7000 Mt in 2020.
- \Box Replacing fossil fuels (gasoline and diesel) with green e-fuels: Hydrogen (H₂).
- \Box Exhaust gas recirculation (EGR) in hydrogen spark ignition engines (H₂SIEs) \rightarrow balance betwenn lean-burn condition performance and low NO_x emissions.
- \Box EGR/IGR can impact combustion \rightarrow residual species such as nitric oxide (NO) and nitric dioxide (NO₂).
- \Box Crucial to study the impact of NO, on lean H₂/air ignition delays under H₂SIE conditions and validate kinetic mechanisms.

Experimental facility and methodology: Laser Gas Analyzer DURAG

- Fast interconversion of NO into NO₂: 2 NO + O₂ = 2 NO₂ [2].
- □ Final mixture composition in the tank vessel measured using a precalibrated multi-compo laser infrared spectrometer LaserCEM.
- \Box Measurement uncertainty for NO and NO₂ is \pm 5 ppm.
- Experiment repeated three times for each mixtures : $H_2/air/NO_x$ (= 50, 250 and 1250 ppm) at ϕ = 0.4.



(b)

2000

1500

2500

Experimental rig and methodology: Rapid Compression Machine

- □ IDT = time difference between the time of the maximum pressure rise rate and the pressure at the end of the compression.
- Crevice to prevent vortex roll-up formation.
- **Conditions:** $\phi = 0.4 p_{c} = 30 60$ bar.
- □ NO_x addition: 50 ppm, 250 ppm and 1250 ppm.
- □ Non-reactive experiments conducted to considers
- Pneumatic System Hydrauli

Crevice

Figure 1. Laser Gas Analyzer DURAG

Phase NO conversion



Figure 3. Comparison of NO and NO₂ mole fractions evolution during the mixing in the RCM tank vessel at p = 5 bar and T = 333 K.

□ Kinetic mechanisms show a faster interconversion with initial NO concentration

the heat losses. Figure 2. RCM from Orléans university

Ignition delay times measurement







increases.

A plateau is reached after 30 minutes.

□ Three final mixtures:

(a) $X_{NO} = 8$ ppm et $X_{NO2} = 42$ ppm; (b) X_{NO} = 9 ppm and X_{NO2} = 241 ppm; (c) $X_{NO} = 11$ ppm and $X_{NO2} = 1239$ ppm

Sensitivity analysis

(R11) $H + O_2 (+ M) \rightleftharpoons HO_2 (+ M)$ (R120) $NO_2 + H \rightleftharpoons NO + OH$ (R4) $H_2 + OH \rightleftharpoons H_2O + H$ (R19) H_2O_2 (+ M) \rightleftharpoons 2 OH (+M) (R18) 2 HO₂ \rightleftharpoons H₂O₂ + O₂ (R21) $H_2O_2 + H \rightleftharpoons HO_2 + H_2$ (R122) $NO_2 + HO_2 \rightleftharpoons HONO + O_2$ (R17) 2 HO₂ \rightleftharpoons 2 OH + O₂ \models Reactivity decreases Reactivity increases (R124) HONO $(+M) \rightleftharpoons NO + OH (+M)$ $X_{\rm NO_x} = 1250 \text{ ppm}$ $X_{\rm NO_x} = 250 \text{ ppm}$ $X_{\rm NO_x} = 50 \ \rm ppm$ (R1) $H + O_2 \rightleftharpoons O + OH$ $X_{\rm NO_x} = 0 \ \rm ppm$

Figure 4. Ignition delay times of $H_2/O_2/N_2/NO_x$ \blacksquare H₂/Air • $H_2/Air/NO_x$ ($X_{NOx} = 50$ ppm) mixtures at φ = 0.4. Ignition delay times decrease with NO_x addition. • $H_2/Air/NO_x$ ($X_{NOx} = 250$ ppm) \land H₂/Air/NO_x (X_{NOx} = 1250 ppm) —Present model The proposed model shows very good agreement - - Aljohani et al. [4]for X_{NOx} = 50 ppm and X_{NOx} = 250 ppm. \dots Sun et al. [3] ----- GRI-Mech 3.0 [5] Discrepancies arise for the case $X_{NOx} = 1250$ ppm.



-6 -12OH sensitivity, s [-]

Figure 5. Sensitive reactions on OH radical for $H_2/air/NO_x$ mixtures for $X_{\rm NOx}$ = 0 ppm, 50 ppm, 250 ppm, 1250 ppm at $p_{\rm C}$ = 50 bar, and $T_{\rm C}$ = 908 K.

 \Box The HO₂/H₂O₂ sequence is not the exclusive contributor to OH production. \Box Recycling loop between NO and NO₂ contributing to a more important production of OH. Reactivity enhancement and this ignition delay times decrease.

OH sensitivity, s [-]

Figure 6. Sensitive reactions on OH radical for $H_2/air/NO_x$ mixtures for $X_{\rm NOx}$ = 0 ppm, 50 ppm, 250 ppm, 1250 ppm at $p_{\rm C}$ = 50 bar, and $T_{\rm C}$ = 908 K.

- \Box Dissociation reaction 2HO₂ = 2OH + O₂ [6] \rightarrow enhance the reactivity of the mixture.
- \Box Recent NO_x sub-mechanism has to be revisited by considering (R17).

Conclusion and perspectives

- \Box Ignition delay times for lean H₂/O₂/N₂/NO_x mixtures under H₂SIEs condition measured using a RCM.
- The NO interconversion into NO₂ measured using a laser gas analyser DURAG and also estimated numerically using different kinetic mechanisms.
- \Box This study shows that ignition delay times decrease with NO_x addition due to a recycling sequence between NO and NO₂, leading to enhanced reactivity \rightarrow OH production. \Box The proposed model displays very good agreement for low-to-moderate NO_x mole fractions.
- \Box Recent NO_x sub-mechanism needs to be revisited by considering the reaction 2HO₂ = 2OH + O₂ [6] to reduce discrepancies at high NO_x mole fractions and high-pressure.
 - [1] Y. Song et al. Energ. Fuels (2020). [4] K. Aljohani et al. Combust Flame (2024). [2] A.B. Sahu et al. Combust. Flame (2022). [5] G.P. Smith et al. http://www.me.berkeley.edu/gri mech/ [3] W. Sun et al. Combust. Flame (2022). [6] S.J. Klippenstein et al. Combust Flame (2022).

