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Potential of water addition in ammonia spark ignition engines

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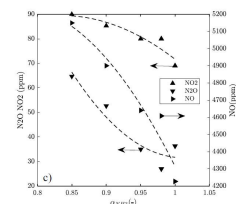
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Background & Objectives

Background :

- Not optimum combustion characteristics of Ammonia (NH₃) induces high compression ratio, boosted conditions or combustion improved to ensure all operating map in SI engine
 - Hydrogen (H₂) is the best combustion improver as it can be produced on board with reformer
 - Drawback remains : NO_x, N₂O and NH₃ at the exhaust (for instance [1] ER = 0.9, p = 1bar, 1000 rpm, α_{NH₃} = level of dissociation)



- EGR and Water injection = one active way to limit thermal NO_x
 - EGR strongly limited in ammonia engine [2]
 - No experimental studies about water injection up today

[1] Mercier et al., Fuel Communications, 11, 2022

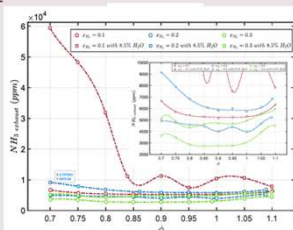
[2] Mounaïm-Rousselle et al. Energies. 2021; 14(14):4141

Objectives :

- First study to evaluate the potential of small water vapor addition
 - In a single cylinder spark-ignition engine
 - 3 different ammonia/hydrogen blends (10, 20, 30% of H₂)
 - from lean to rich NH₃/H₂/air blend
- Provide first analysis with kinetics simulation

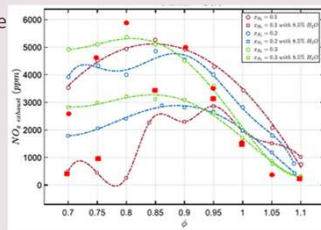
2 Unburnt ammonia

- Important minimum level of unburnt NH₃ = 2800 ppm
- unburnt NH₃ emissions increases by a factor 1.5 with water addition
- but less than 1% for 30 and 20% of H₂ in the blend.
- the best efficiency in terms of combustion for mixtures near the stoichiometry (0.95 to 1.05)



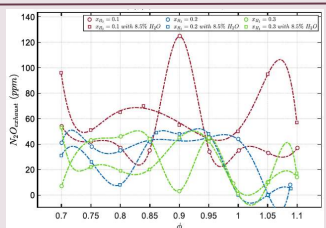
3 NOx and N₂O emissions

- the addition of H₂ yields an increase of NO_x at ER>0.9 but a decrease of NO_x at ER<0.9.
- addition of water, even in small amounts decreases NO_x emissions, more than 45% in lean mixtures as found previously with 8% of N₂ dilution [2].
- Impact reduced but still significant when 0.95 < ER < 1.05



Red filled symbols: simulated NO_x for x_{H₂O}=0.1

- no clear tendencies for N₂O emissions with ER, H₂ or water addition
- except for the lowest H₂ %,
 - all values < 50 ppm (limit of measurement accuracy)
 - lowest emissions around stoichiometry (1 - 1.05).



Experimental Set-up & Numerical tools

Engine characteristics

| | |
|------------------------------------|--------------|
| Displaced volume | 0.535 L |
| Stroke | 115 mm |
| Bore | 77 mm |
| Connecting rod length | 177 mm |
| Compression ratio | 14 |
| Coolant and oil temperature | 80 °C |
| Regime | 1000 rpm |
| p _{int} , T _{in} | 1 atm, 55 °C |

Conditions

- 10, 20, 30% of H₂ in the fuel
- ER: 0.7 to 1.1
- water vapor injection
 - 8.5% vol. substituted in the fuel

Chemkin Pro SI engine model

- Wiebe function, 2 zones
- Classical Washni coefficients

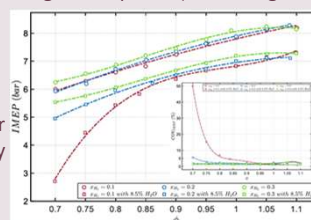
Stagni et al. mechanism [3]

- 31 species and 203 reactions

1 Stability and performance of the engine

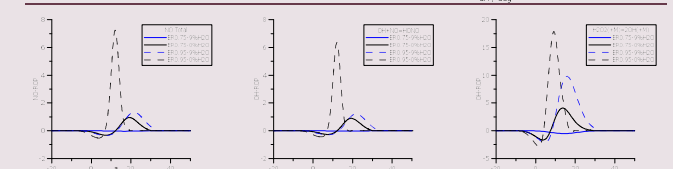
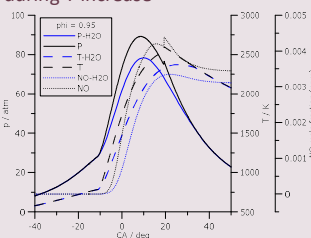
- Very small decrease of input energy (2% max)
- Strong decrease of IMEP even if water in gaseous phase (no cooling effect): 12% in average for 0.9<ER<1.1
 - especially for lowest H₂ content and ER ≤ 0.85 (lost of engine stability σ_{IMEP}>>5%)
 - Combustion slower with water addition: increase of 4 CAD for any H₂%
 - identical combustion duration 30% H₂ with water and 10%H₂w/w water.

IMEP



4 Discussion about NOx with simulated results

- Water addition decrease T_{max} (around 160 K) at both ER, with also p_{max} decrease (23 bar at 0.75 ER and 10 bar at 0.95 ER, due to change of spark ignition timing optimized to reach maximum IMEP).
- Averaged NO species profiles increase during T increase
- Due to high temperature range (T>2100K), most NO are formed through the well-known thermal-NO route
- The fuel-NO route (NH₃>NH₂>NH>HNO>NO) is more efficient at ER=0.75 due the highest OH quantities than at ER=0.95



- without H₂O (black curves), NO species consumed and then formed
- With H₂O (blue curves),
 - At ER= 0.95, NO species first consumed and second formed,
 - At ER=0.75, NO species are only slightly consumed.
- NO-ROP for reaction OH+NO⇌HONO are similar of the total NO for 4 studied cases
- Total OH-ROP analysis indicates OH radicals consumed for 4 studied cases
- but OH-ROP for reaction H₂O₂(+M)⇌2OH(+M) presents similar tendencies with a specific consumption of OH at ER=0.75 with H₂O
 - not only pressure-dependent but also third-body efficient dependent. Water substitution affects OH formation and therefore NH₃ and H₂ oxidation

Conclusions & perspectives

- First experimental study about the potential of water addition in NH₃/H₂ fuel to reduce NO_x emissions
- For lean NH₃/H₂ mixtures, NO_x strongly reduced by water presence, even if both thermal and fuel NO_x routes are involved, due to change of OH radicals, pointed out by the simulated by OD 2 zone model
- Further experimental studies and kinetic chemistry analysis necessary to discriminate the effect of pressure, temperature and chemistry on the decreasing of NO

Acknowledgements

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