# Potential of water addition in ammonia spark ignition engines

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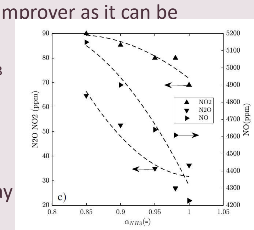
## Background & Objectives

**Background :**

- Not optimum combustion characteristics of Ammonia ($NH_3$) induces high compression ratio, boosted conditions or combustion improved to ensure all operating map in SI engine
  - ➢ Hydrogen ($H_2$) is the best combustion improver as it can be produced on board with reformer
  - ➢ Drawback remains : NOx, $N_2O$ and $NH_3$ at the exhaust (for instance [1] ER = 0.9, $p$ = 1bar, 1000 rpm, $\alpha NH_3$ = level of dissociation)



- EGR and Water injection = one active way to limit **thermal** NOx
  - ➢ 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 $H_2$)
  - ➢ from lean to rich $NH_3/H_2$/air blend
- Provide first analysis with kinetics simulation

## Experimental Set-up & Numerical tools

**Engine characteristics**

| | |
|---|---|
| Displaced volume | 0.535 L |
| Stoke | 115 mm |
| Bore | 77 mm |
| Connecting rod length | 177 mm |
| Compression ratio | 14 |
| Coolant and oil temperature | 80 °C |
| Regime | 1000 rpm |
| $p_{in}$, $T_{in}$ | 1 atm, 55°C |

**Conditions**

- 10, 20, 30% of $H_2$ 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 Woshni coefficients

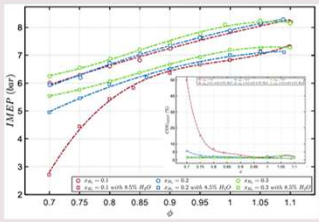
**Stagni et al. mechanism [3]**

- 31 species and 203 reactions

## 1 Stability and performance of the engine

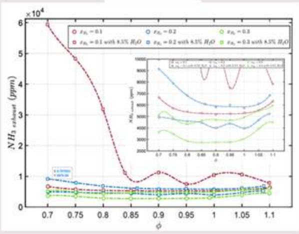
- Very small decrease of input energy (2% max )
- Strong decrease of IMEP even if water in gaseous phase (no cooling effect): 12% in average for 0.9<ER<1.1
- ➢ especially for lowest $H_2$ content and ER ⩽ 0.85 (lost of engine stability $\sigma_{IMEP} \gg 5\%$)
- Combustion slower with water addition: increase of 4 CAD for any $H_2$%
  - ➢ **identical combustion duration 30% $H_2$ with water and 10%$H_2$ w/o water.**

IMEP



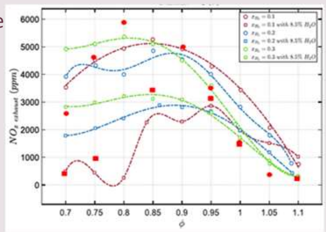
## 2 Unburnt ammonia

- Important minimum level of unburnt $NH_3$ = 2800 ppm
- unburnt $NH_3$ emissions increases by a factor 1.5 with water addition
- **but** less than 1% for 30 and 20% of $H_2$ in the blend.
- the best efficiency in terms of combustion for mixtures near the stoichiometry (0.95 to 1.05)



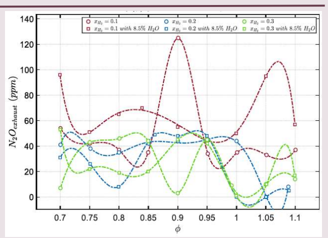
## 3 NOx and $N_2O$ emissions

- the addition of $H_2$ yields an increase of $NO_X$ at ER>0.9 but a decrease of NOx at ER<0.9.
- addition of water, even in small amounts decreases NOx emissions, more than 45% in lean mixtures as found previously with 8% of $N_2$ dilution [2].
- Impact reduced but still significant when 0.95 <ER< 1.05



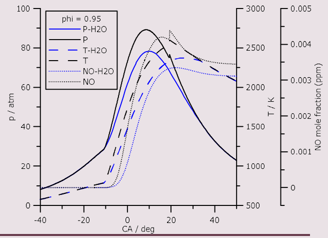
Red filled symbols: simulated $NO_X$ for $x_{H2}$=0.1

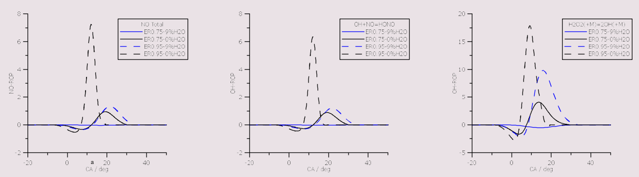
- no clear tendencies for $N_2O$ emissions with ER, $H_2$ or water addition
- except for the lowest $H_2$ %,
  - ➢ all values < 50 ppm (limit of measurement accuracy)
  - ➢ lowest emissions around stoichiometry (1 – 1.05).



## 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** ($NH_3$>$NH_2$>NH>HNO>NO) is more efficient at ER=0.75 due the highest OH quantities than at ER=0.95





- without $H_2O$ (black curves), NO species consumed and then formed
- With $H_2O$ (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 $H_2O_2$(+M)⇌2OH(+M) presents similar tendencies with a specific consumption of OH at ER=0.75 with $H_2O$
  - ➢ not only pressure-dependent but also third-body efficient dependent. Water substitution affects OH formation and therefore $NH_3$ and $H_2$ oxidation

## Conclusions & perspectives

- First experimental study about the potential of water addition in $NH_3/H_2$ fuel to reduce NOx emissions
- For lean $NH_3/H_2$ mixtures, NOx strongly reduced by water presence, even if both thermal and fuel NOx routes are involved, due to change of OH radicals, pointed out by the simulated by 0D 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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