

# CH<sub>3</sub>OH/NH<sub>3</sub> Mixture: A Possible Green Energy

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## Summary

Given the current problems with conventional fossil fuels, the study of the oxidation of more environmentally friendly fuels is on the rise. The oxidation of ammonia combined with oxygenated organic compounds could be a viable solution in the future to replace the most polluting fuels.

## Introduction

Emissions from conventional fossil fuels are currently affecting critically the environment, increasing the greenhouse effect and, consequently, climate change. An alternative to conventional fuels could be ammonia. Ammonia is a large storage of hydrogen. Furthermore, the NH<sub>3</sub> storage technology is widely developed due to its extensive use in the fertilizer industry. So, a migration to ammonia as the main fuel would be easy. Additionally, it is possible to synthesize ammonia sustainably, by using renewable energies such as wind energy or photovoltaics [1]. The power-to-fuel strategy can be followed, with excess energy from renewable energy being used (green ammonia).

However, the combustion of NH<sub>3</sub> has some disadvantages, such as a low flammability limit, high ignition energy, low energy density and potentially high NO emissions [2]. One of the strategies to counteract these problems is the use of mixtures with improved ignition properties. One of the candidates for this mixture may be methanol (CH<sub>3</sub>OH). The ignition parameters of CH<sub>3</sub>OH are promising, having a high-octane rating, low flammability and high heat absorption, which can help to improve engine cooling. At the same time, it favours lower emissions of NO<sub>x</sub>, CO and soot compared to conventional fuels. And, as with NH<sub>3</sub>, it can be produced with little environmental impact, using biomass, renewable energy or CO<sub>2</sub> recycling.

## Experimental

The experiments have been carried out using a quartz flow reactor. The reactor, with an internal diameter of 8.7 mm and 200 mm long, is placed within an

electrically heated oven [3]. A Type-K fine-wire thermocouple is used to measure the isothermal conditions achieved ( $\pm 5$  K). A 1000 mL·min<sup>-1</sup> (STP) gas flow rate is used. Both NH<sub>3</sub> and CH<sub>3</sub>OH have an initial concentration of 500 ppm. Every gas reactant is added individually.

Temperature, excess oxygen ratio ( $\lambda$ ), NH<sub>3</sub> and DME have been varied in these experiments.  $\lambda$  (defined as the O<sub>2</sub> fed divided by the stoichiometric oxygen) was changed for each experiment (0-2). Conditions are shown in Table 1. Each experiment was run in a range of temperatures between 875-1425 K. A gas chromatograph Agilent 990 Micro GC equipped with TCD and FID detectors is used to measure CO, CO<sub>2</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>, NH<sub>3</sub>, N<sub>2</sub>O, H<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, HCN, CH<sub>3</sub>CHO and CH<sub>3</sub>OH. In addition, the outlet gas stream is also analyzed by an Advance Optima AO2020 series continuous gas analyzer, which measures the concentration of NO.

Tabla 1. Experimental conditions

CH <sub>3</sub> OH, ppm	NH <sub>3</sub> , ppm	$\lambda$	t <sub>r</sub> (s)
511	497	0	191/T(K)
509	482	0.5	190/T(K)
493	461	1	192/T(K)
530	486	1.9	190/T(K)

An updated mechanism based on the work of Glarborg et al. (2018) [4]. The simulations have been carried out using the Chemkin-Pro 2023 software, with the Pug Flow Reactor (PFR) module.

## Results and discussion

Figure 1 shows the conversion of both ammonia and methanol as a function of the temperature for different stoichiometries. The  $\text{NH}_3$  consumption is influenced by the initial oxygen used, and it is noted that under fuel-rich conditions the ammonia is not completely consumed. This means that the interaction of oxygen and its derived radicals is predominant. When  $\text{O}_2$  is increased, ammonia is consumed in the narrow temperature range of 1100-1250 K.

Concerning  $\text{CH}_3\text{OH}$ , it is deduced that the presence of  $\text{O}_2$  accelerates its conversion since its thermal decomposition is slower than the oxidation ones. At the initial consumption temperatures, a higher conversion for fuel-rich conditions is noted, which may lead to an inhibition caused by ammonia. This is due to competition for OH, H and O radicals.

## Conclusion

In this work, the conversion of an  $\text{NH}_3/\text{CH}_3\text{OH}$  mixture is studied as a function of  $\lambda$ , and it is concluded that fuel-lean conditions favour the oxidation of both fuels. Furthermore, the presence of  $\text{CH}_3\text{OH}$  favours the oxidation of  $\text{NH}_3$ , while  $\text{CH}_3\text{OH}$  conversion is inhibited at the onset of the reaction under fuel-lean conditions.

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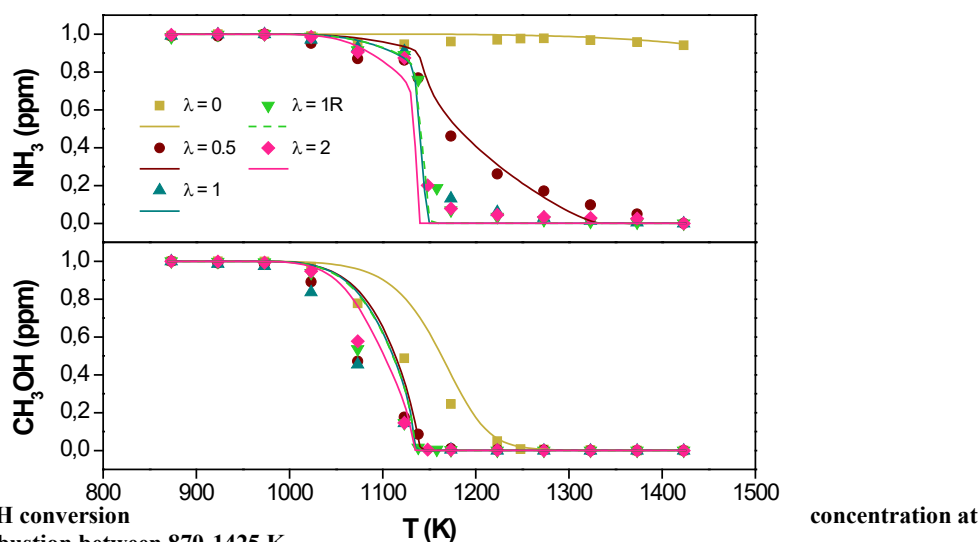


Figure 1.  $\text{NH}_3$  and  $\text{CH}_3\text{OH}$  conversion temperature combustion between 870-1425 K.