Effect of Water on the Auto-Ignition of a Non-Carbon Nitrogen-Based Monofuel

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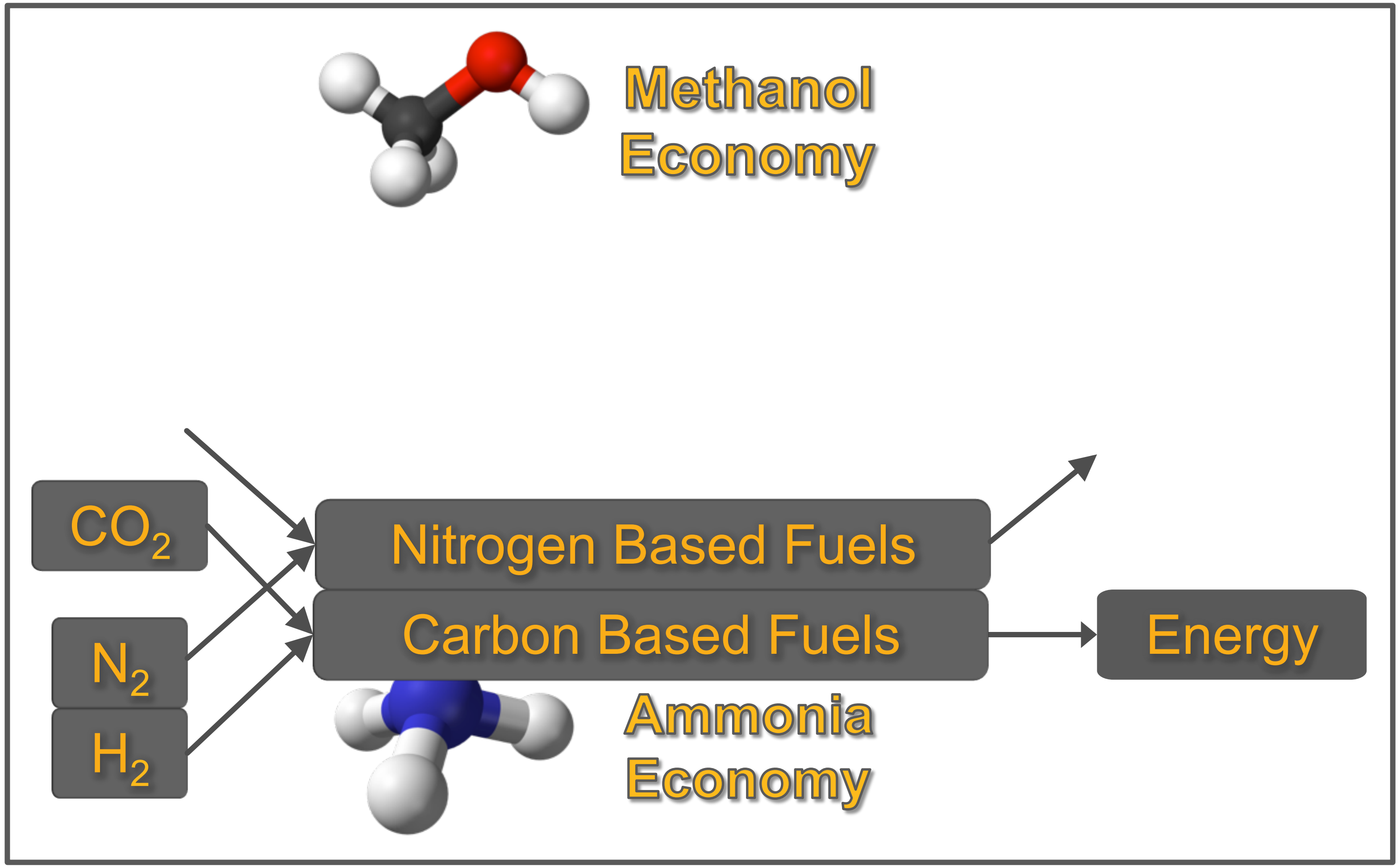
01/11/2017

AIChE 2017

Motivation

- Economical availability of renewable H_2 is getting closer
- H_2 is incompatible with fuel transport infrastructure
- Chemical fuels are attractive H_2 carriers since they are safer and easier to transport
- Chemical fuels offer higher volumetric energy densities than pure H_2

But what fuels can we choose from?

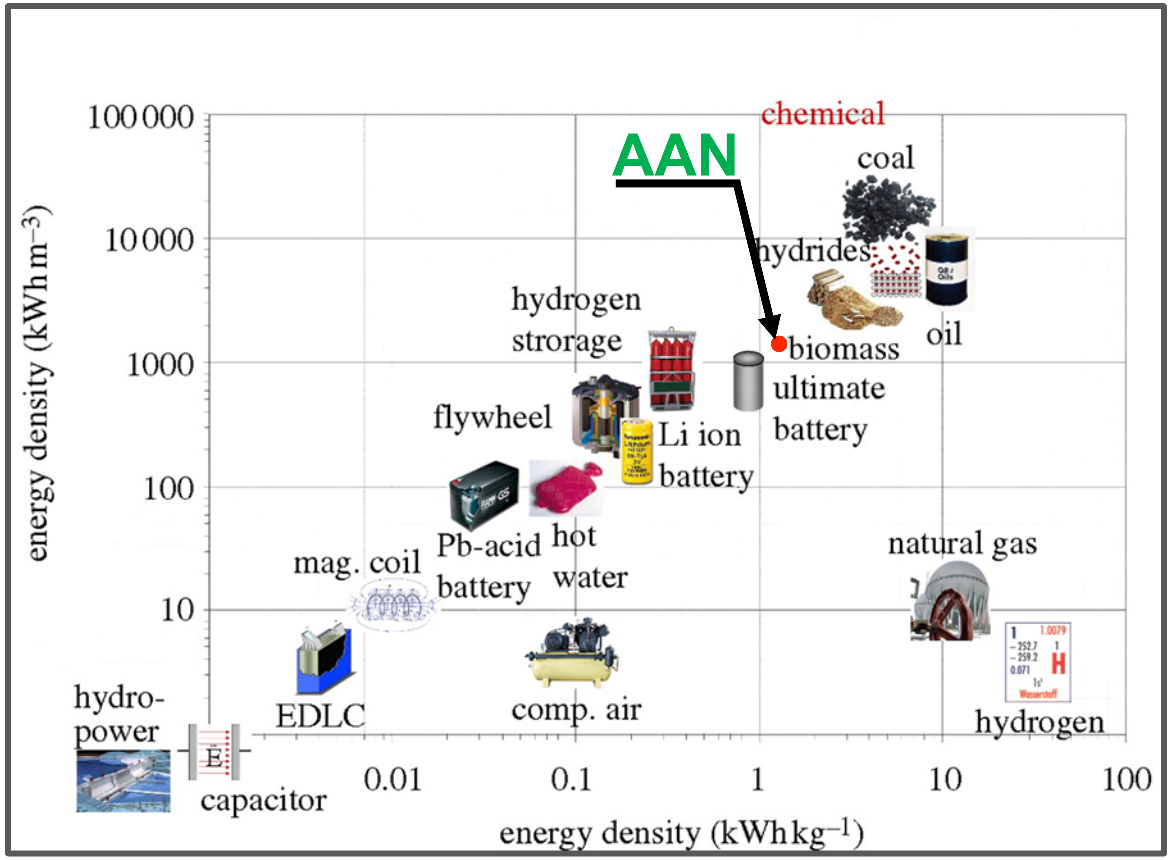


Introduction

- Aqueous ammonia/ammonium nitrate (AAN) is a **carbon free** nitrogen-based monofuel
- Composed from mass-produced fertilizers
- Principal combustion products are N_2 and H_2O:

$$3NH_4NO_{3\,(aq)} + 2NH_4OH_{\,(aq)} + 4H_2O \rightarrow 4N_2 + 15H_2O$$

- Volumetric energy density close to CNG at distribution pressure
- Compatible with current fuel infrastructure
- **No PM, VOC, CO_2 and CO emissions**



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Introduction

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- The thermal autoignition of AAN occurs in the **gas phase**
- Ammonium nitrate thermally decomposes under heating:

$$NH_4NO_{3\,(aq)} \rightarrow NH_{3\,(g)} + HNO_{3\,(g)}$$

- Ammonia and water evaporate into the gas phase
- Four principal homolytic reactions known from literature:

$$HNO_3 \rightarrow OH + NO_2$$

$$NH_3 + OH \leftrightarrow NH_2 + H_2O$$

$$NH_2 + NO_2 \rightarrow N_2O + H_2O$$

$$NH_2 + NO_2 \rightarrow H_2NO + NO$$

- We recently showed other nitric acid / ammonia reactions might be significant:

$$HNO_3 + HONO \rightarrow H_2O + N_2O_4$$

$$N_2O_4 + M \rightarrow 2NO_2 + M$$

$$NH_3 + NO_3 \rightarrow HNO_3 + NH_2$$

Fuel Processing Technology

B. Mosevitzky, G.E. Shter, G.S. Grader, Fuel Process. Technol. 159, 363–368, 2017.

Introduction

- Ammonium nitrate is a net oxidizer, decomposing into NH_3 (reducer) and HNO_3 (oxidizer):

$$3NH_4NO_{3(aq)} + 2NH_4OH_{(aq)} + XH_2O_{(l)} \rightarrow$$
$$3HNO_{3(g)} + 5NH_{3(g)} + (X+2)H_2O_{(g)} \rightarrow$$
$$4N_{2(g)} + (X+11)H_2O$$

- The combustion of stoichiometric AAN does not require O_2/Air.
- Changing the water content of AAN affects the solubility of the components in the aqueous mixture.
- Therefore, more water can be added to ensure a liquid solution even at subzero temperatures.

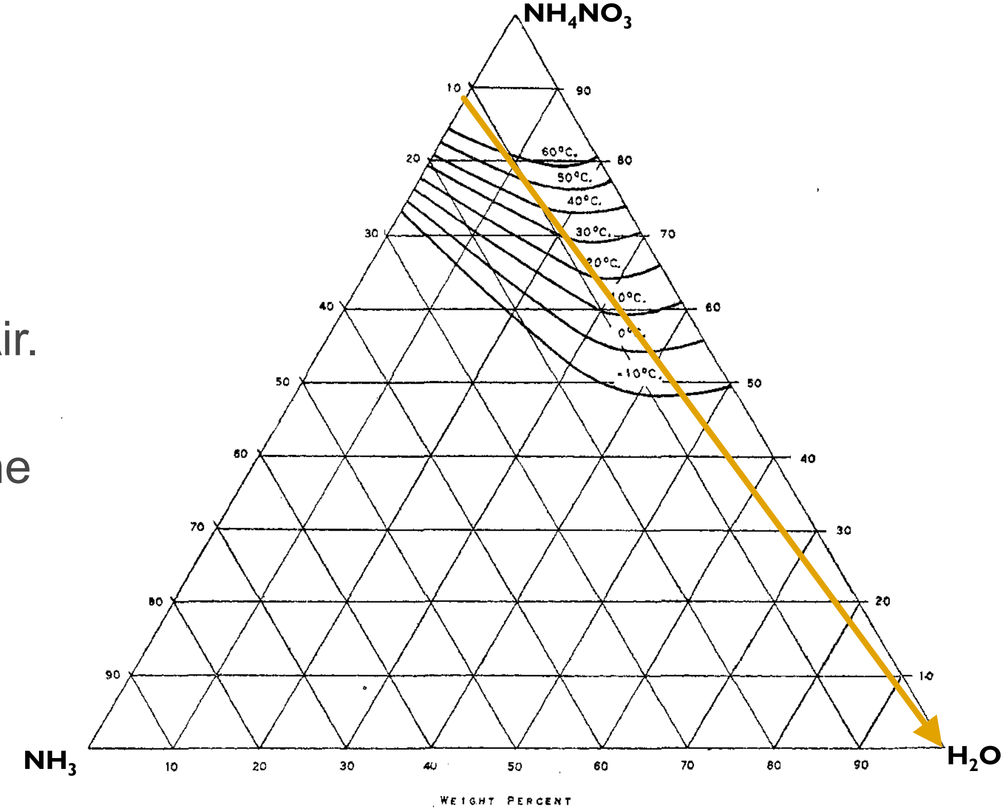

Figure 1. Solubility in the System Ammonium Nitrate–Ammonia–Water

Introduction

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- The autoignition temperature (AIT) is the lowest temperature from which the fuel can ignite without the need for additional external energy
- Used to identify how various parameters affect the thermal autoignition
- The parameter we used in this study to observe changes in the autoignition process as well as validate the model we used

Goals

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Main goals

What effect does changing the water content of AAN have on the AIT?

What is the cause of the observed effect?

Results and Discussion

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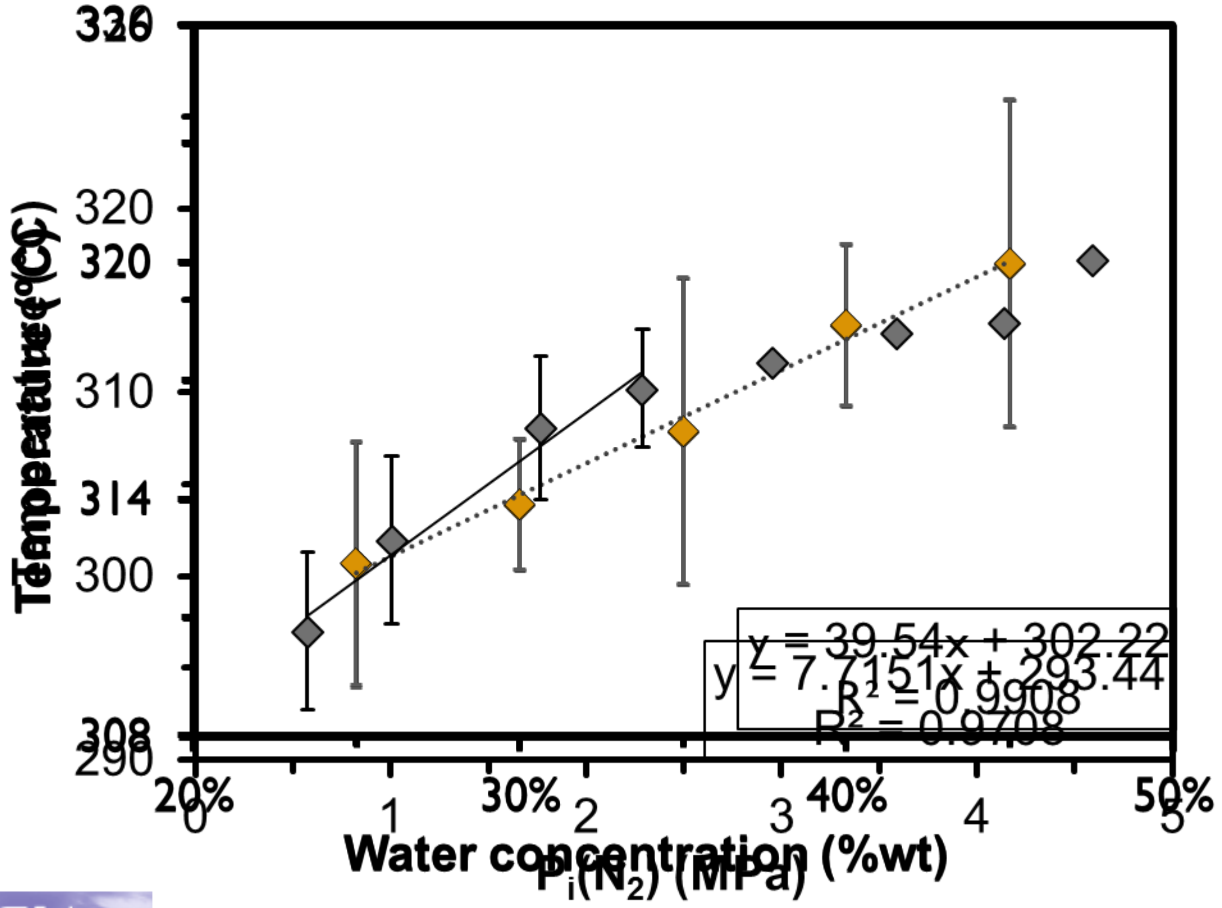
- The AIT increased with the water content
- Thermal autoignition was detected for all tested samples
- A linear increase in AIT was observed
- Linear behavior was previously observed at low diluent (N_2) pressures

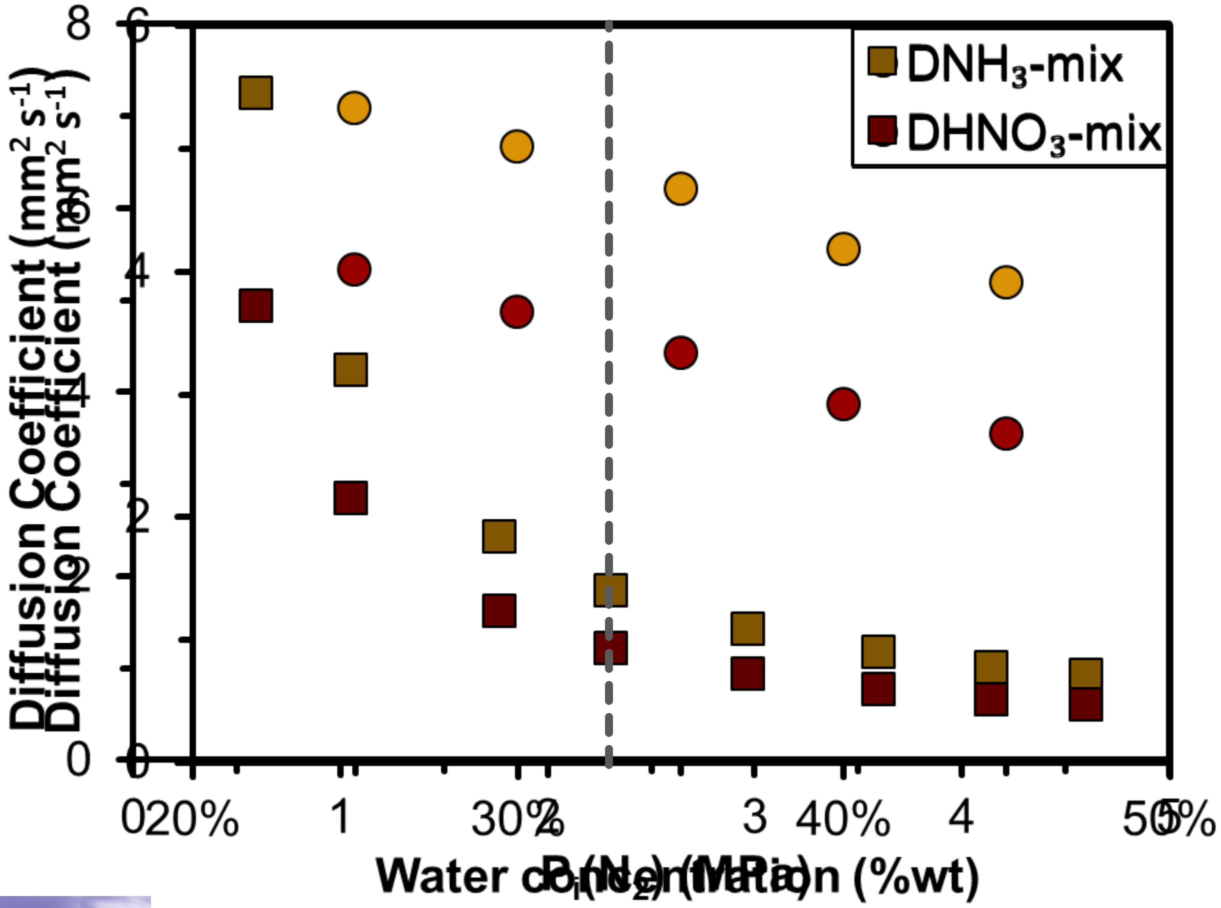


B. Mosevitzky, G.E. Shter, G.S. Grader, Fuel Process. Technol. 159, 363–368, 2017.

Results and Discussion

- This linear behavior was previously found to characterize the thermal autoignition at high diffusion conditions (D>1.5 mm^2 s^{-1}).

- The diffusion coefficients of both HNO_3 and NH_3 were above 2.5 mm^2 s^{-1} at all tested water contents

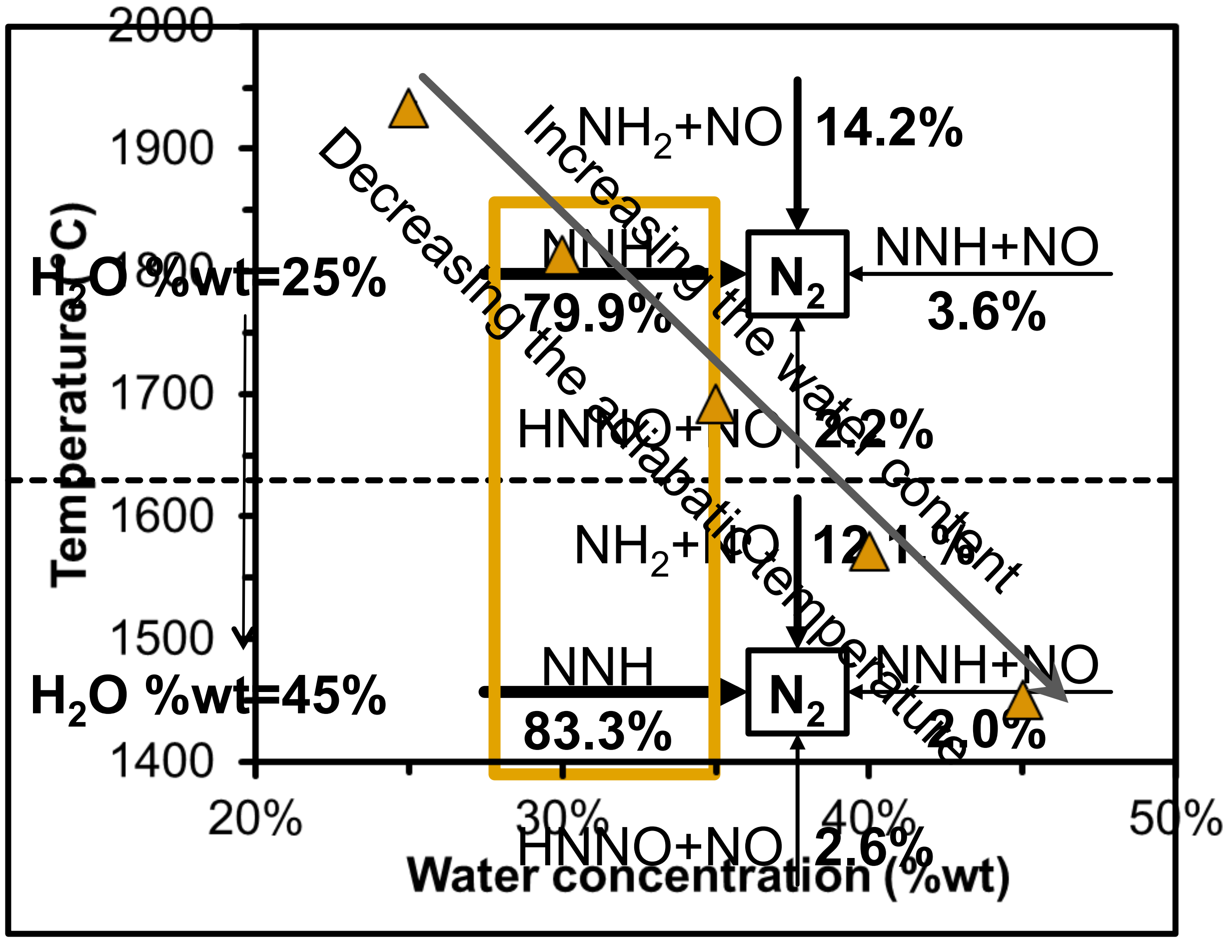


B. Mosevitzky, G.E. Shter, G.S. Grader, Fuel Process. Technol. 159, 363–368, 2017.

Results and Discussion

But what causes the increase in AIT?

- Added water could affect pressure-dependent reactions (three-body reactions).
- The additional water acts as a heat sink.

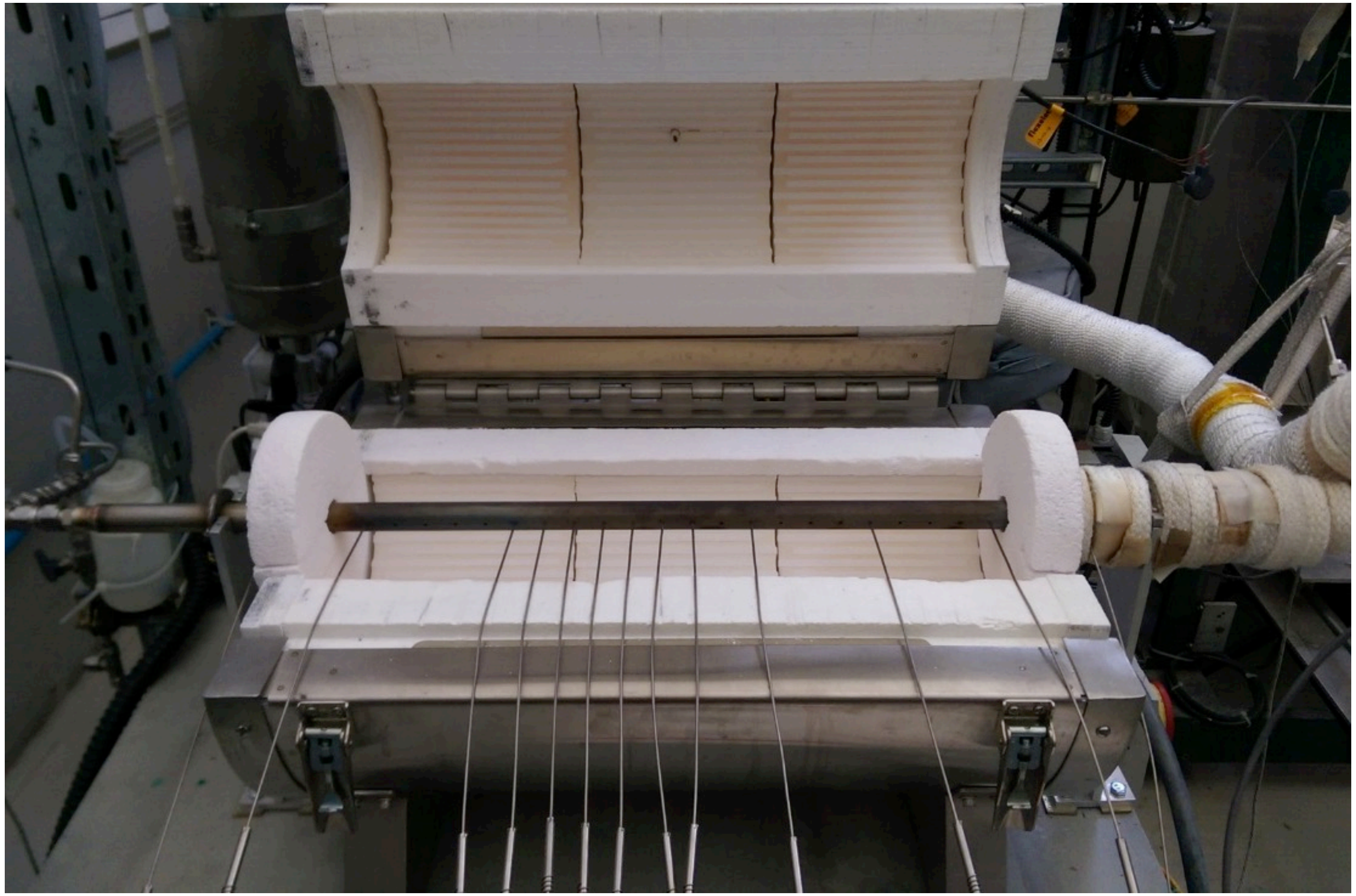


Conclusions

- Adding up to 45%wt water to AAN still allows thermal autoignition.
- The AIT value increased linearly with AAN water content.
- This linear behavior is linked to large mass diffusion coefficients.
- The increase in AIT was attributed to two main sources:
  - Possible effect of pressure-dependent reactions.
  - Increased diluent (water) content acting as a heat sink.

Future Work

- Addition of oxygen instead of AN to work at high ϕ values (batch and continuous combustion)
- Effects of pressure / temperature / water content / equivalence ratio on AAN continuous combustion



Acknowledgements

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The Ed Satell Family Nitrogen-Hydrogen Alternative Fuels (NHAF) Reaction Research Laboratory

Relevant Publications

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