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Reaction Class-Based CHON Combustion Mechanism Development

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[1]Physico-Chemical Fundamentals of Combustion
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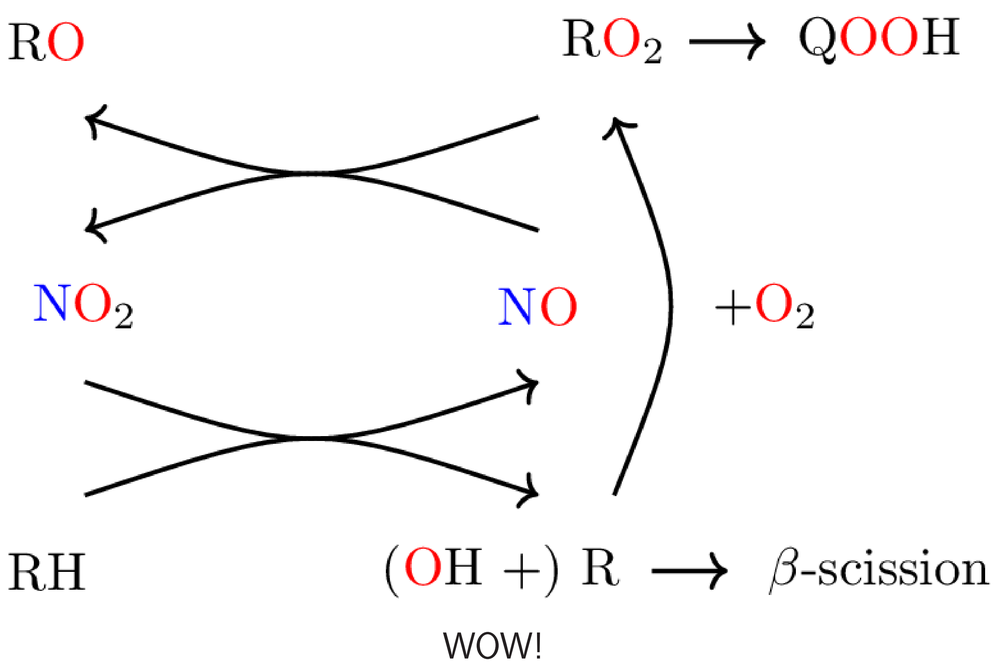
Introduction

- Interactions of NO_x (NO and NO_2) with the combustion process are increasingly relevant in engines with exhaust gas recirculation (EGR) and/or alkyl nitrate cetane enhancers
- Low-temperature combustion reactions with nitrogen are not well-studied and may have significant effects
- Sustainable fuels, produced from bio-based carbon feedstocks, CO_2 , and renewable electricity, contain additional functional groups whose reactions with NO_x are not well-characterized

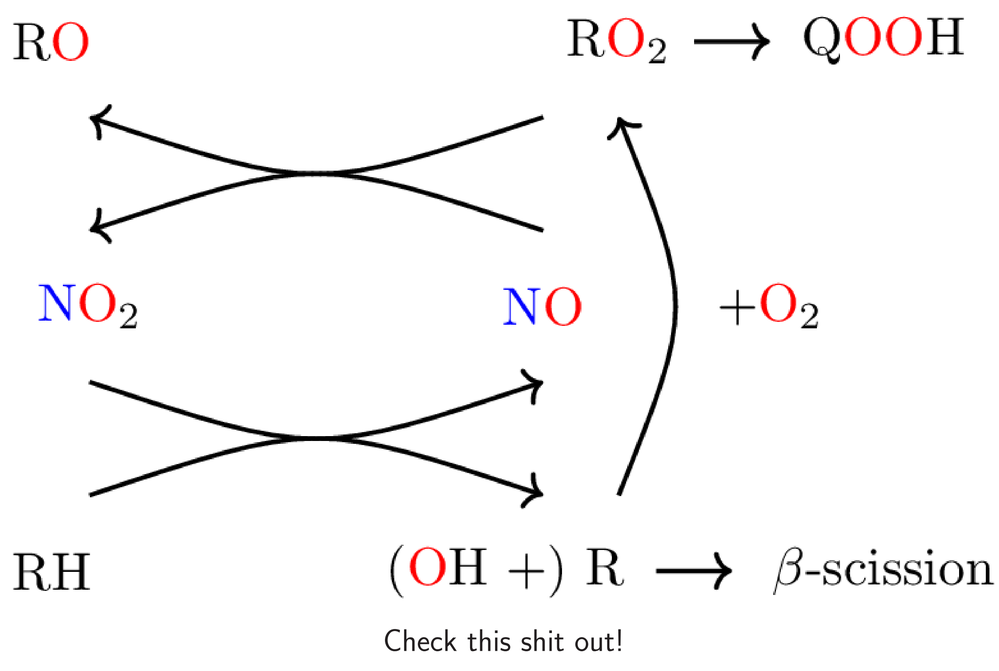
Model Development

- Pentane isomer mechanism (CHO) of Bugler *et al.* utilized as C_0-C_5 base mechanism
- A sample citation[1]

Modeling results

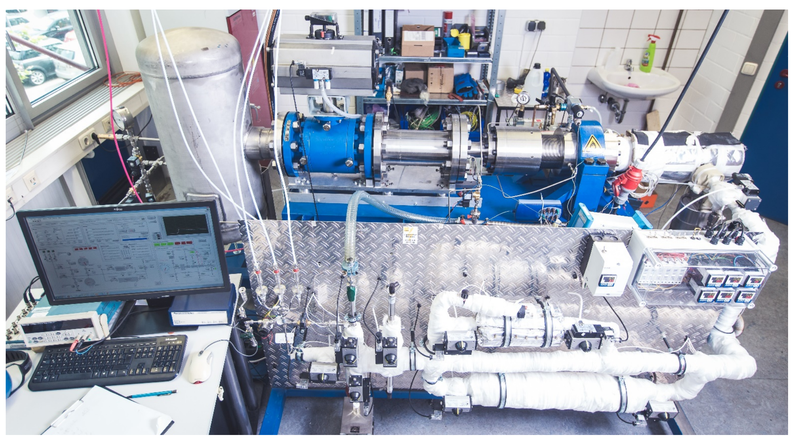


WOW!

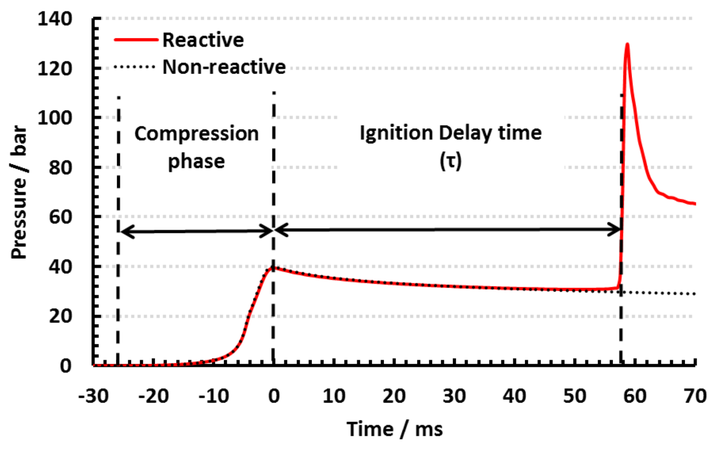


Check this shit out!

Rapid Compression Machine (RCM)



PCFC RCM Facility



Characteristic RCM ignition experiments

- Ignition delay time (IDT) measurements 2 to 200 ms
- Variable compression ratio 9 - 32
- End-of-compression pressure up to 100 bar, peak 1000 bar allowed

Work-in-progress

Ab initio calculations

REFERENCES

[1] M. E. Fuller DOI: 10.1016/j.enconman.2014.08.015.