

# Reaction Class-Based CHON Combustion Mechanism Development

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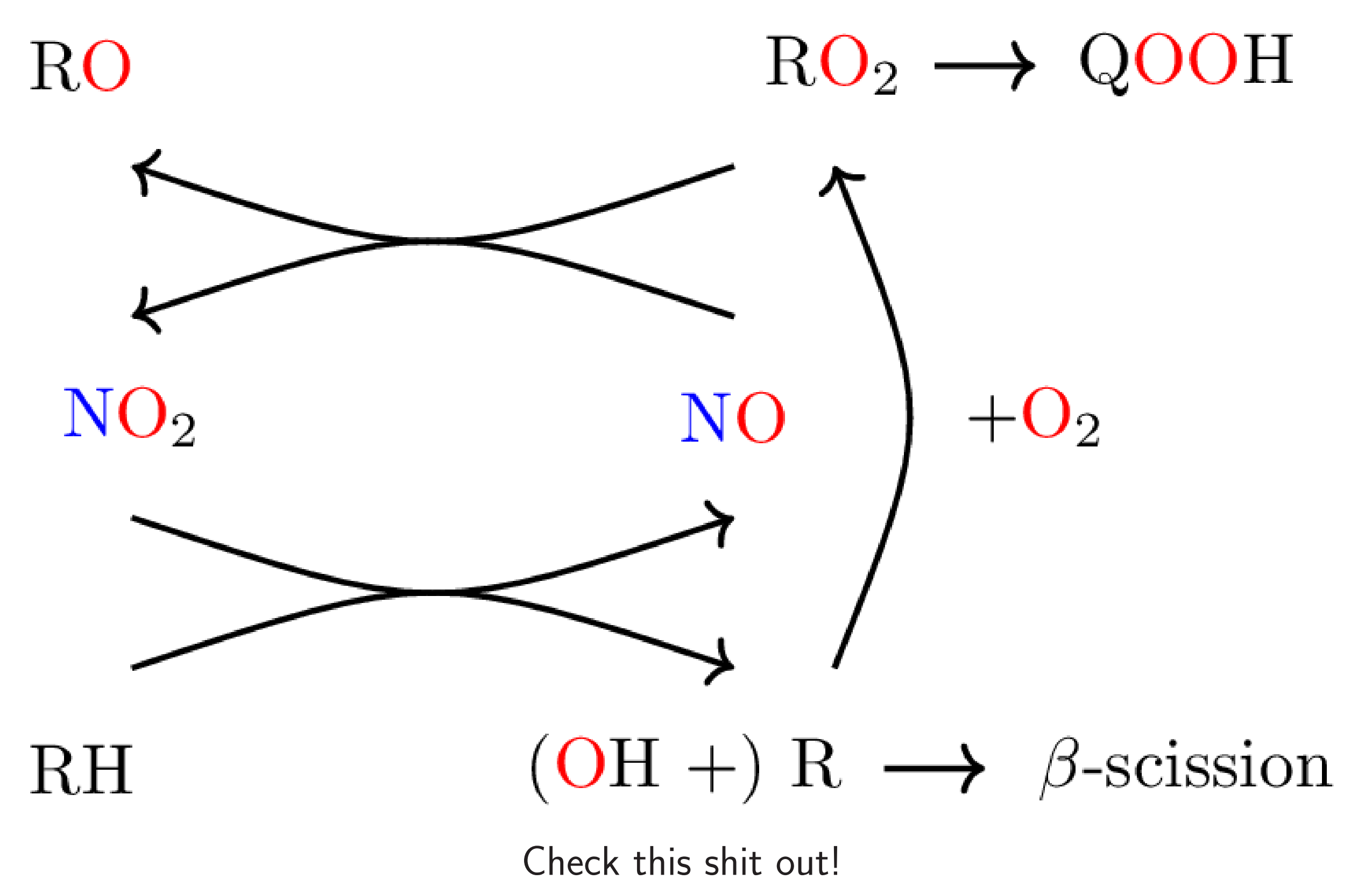
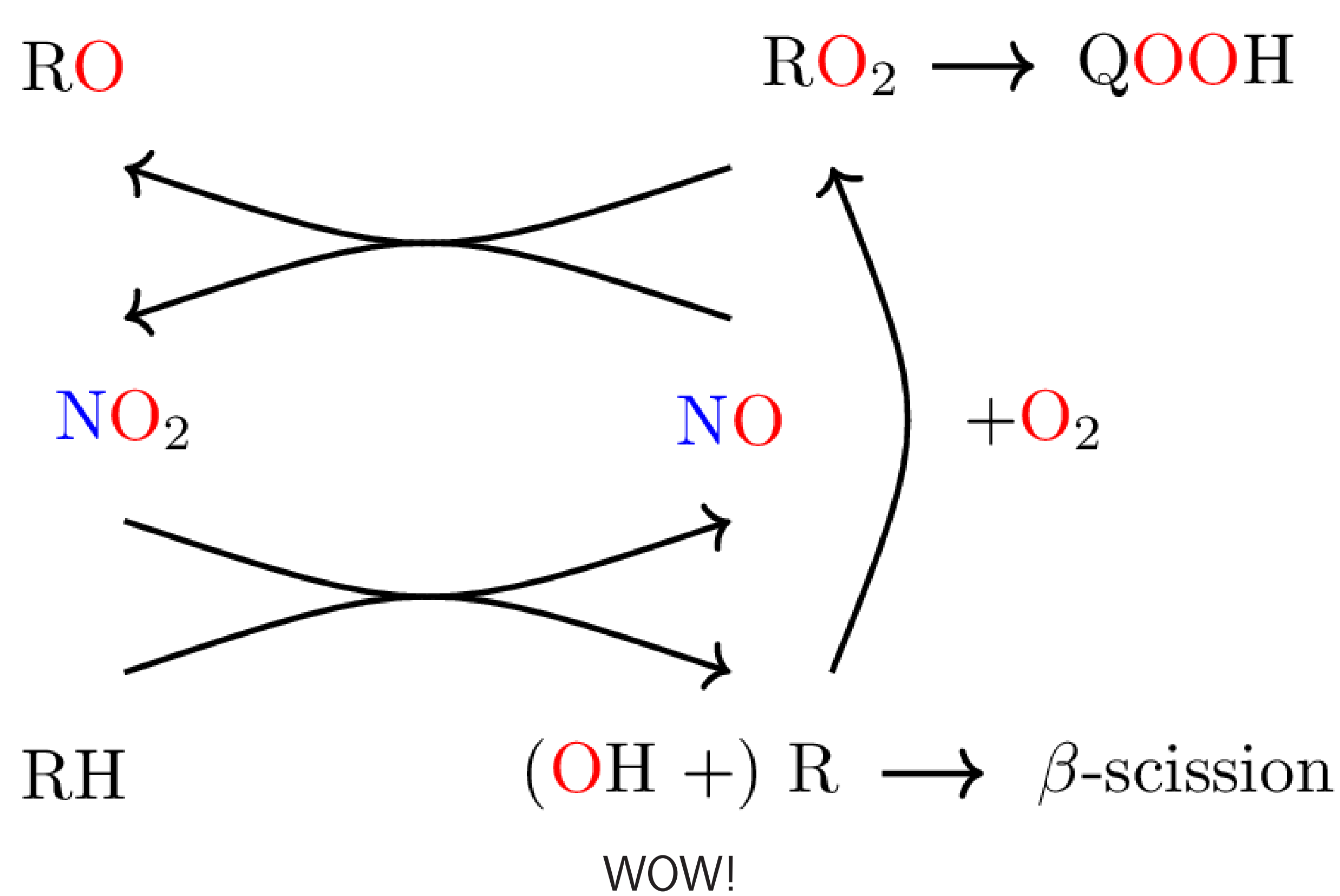
## Introduction

- Interactions of NO<sub>x</sub> (NO and NO<sub>2</sub>) 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<sub>2</sub>, and renewable electricity, contain additional functional groups whose reactions with NO<sub>x</sub> are not well-characterized

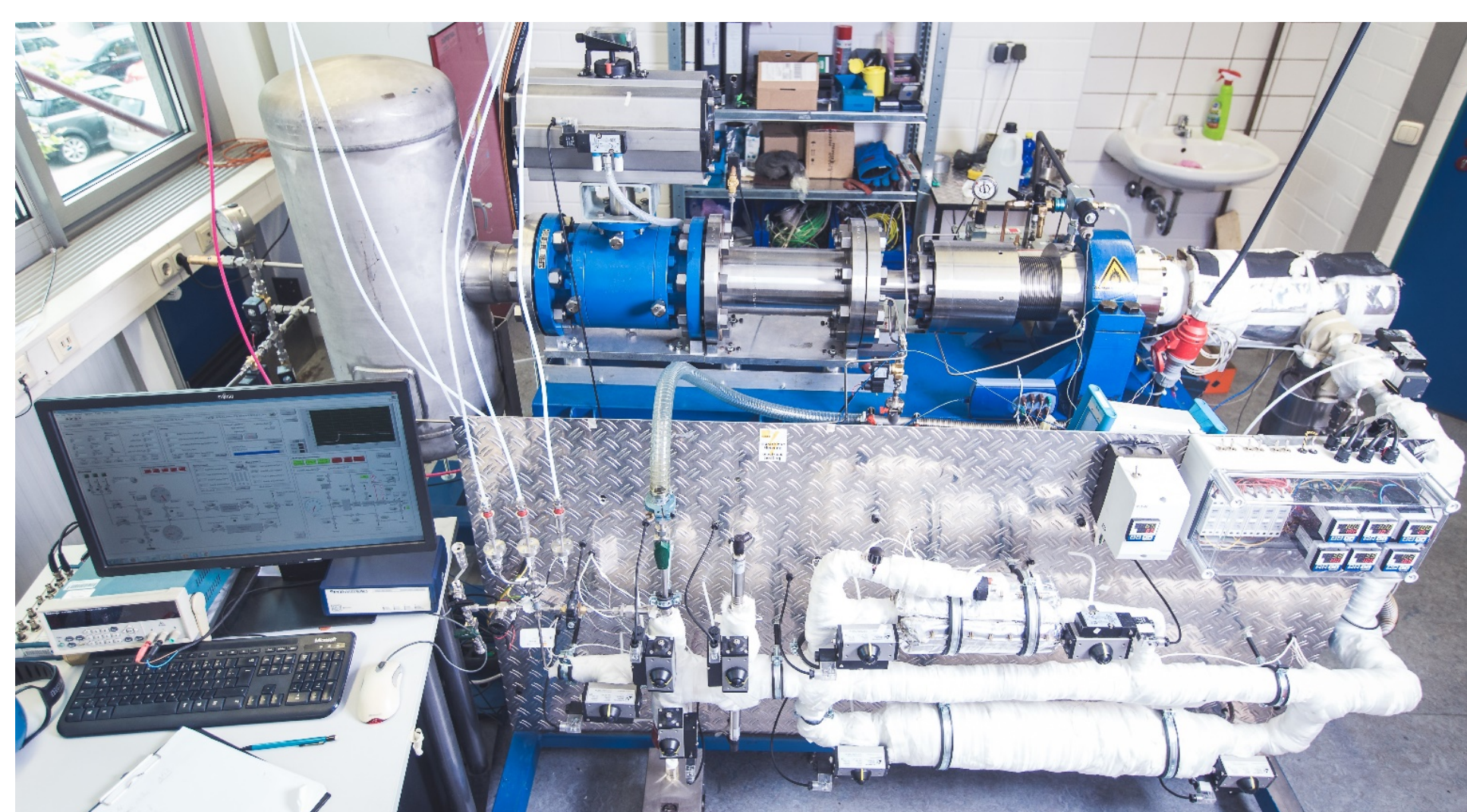
## Model Development

- Pentane isomer mechanism (CHO) of Bugler *et al.* utilized as C<sub>0</sub>-C<sub>5</sub> base mechanism
- A sample citation[1]

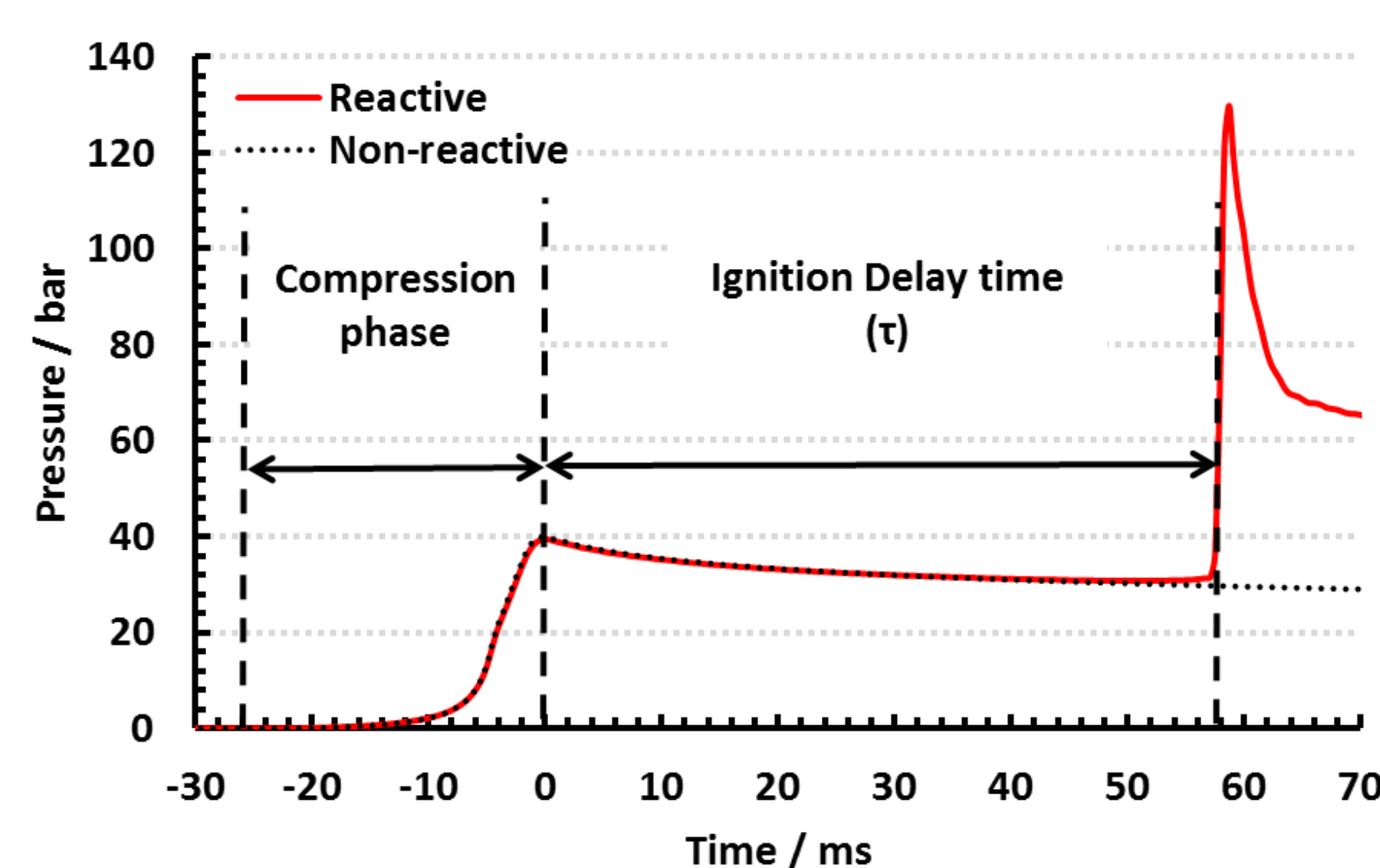
## Modeling results



## 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.