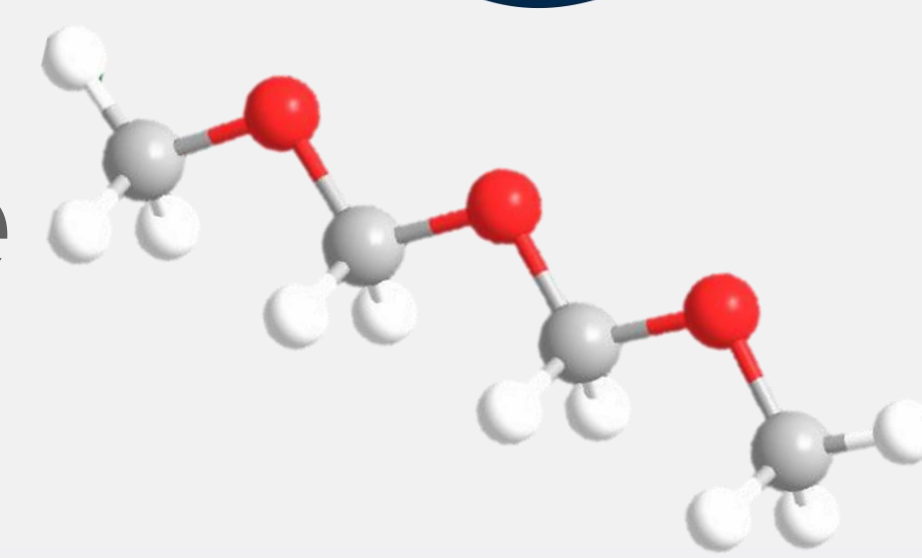


A combined experimental and kinetic modeling study on the low-temperature oxidation of oxymethylene ether-2 (OME-2)



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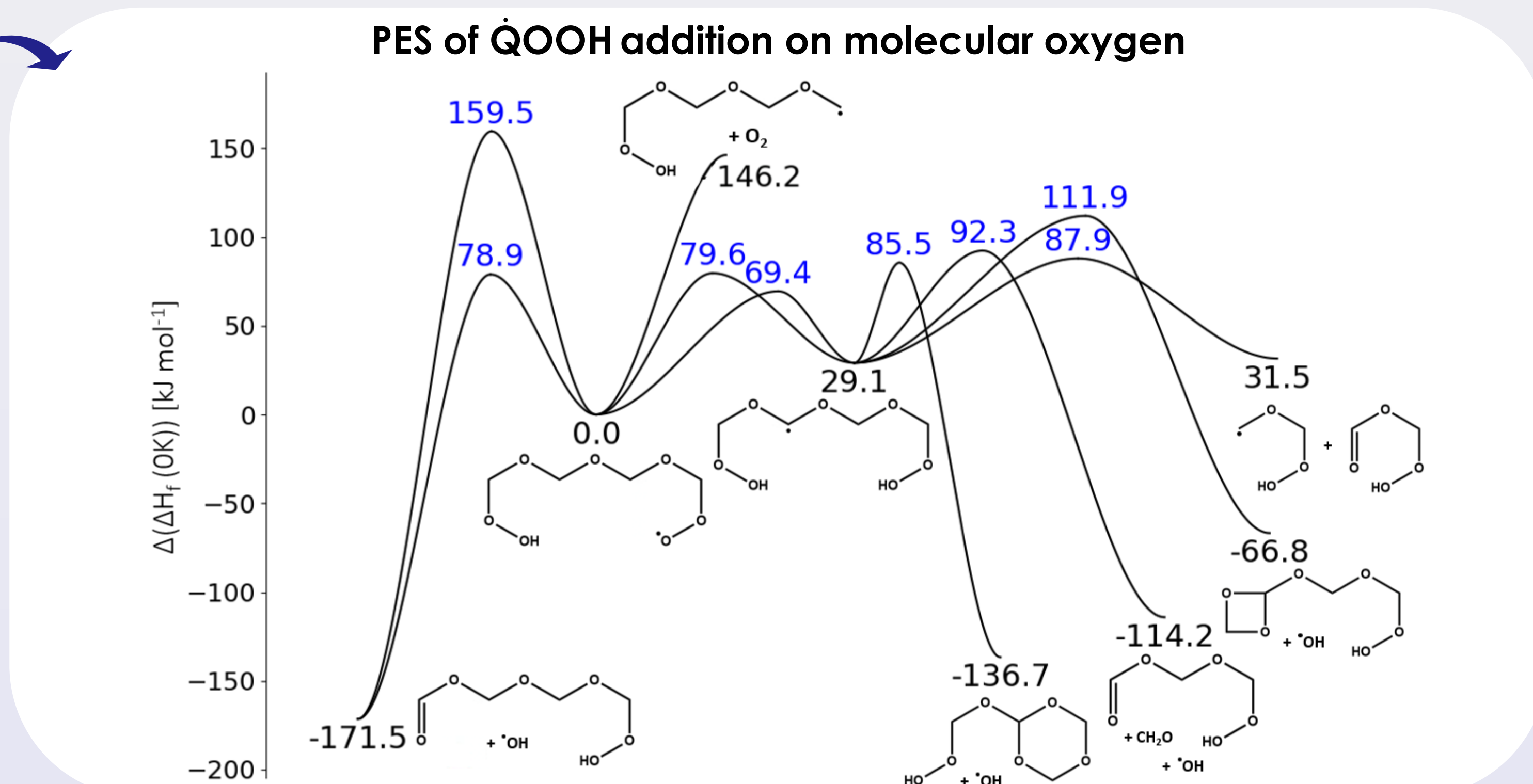
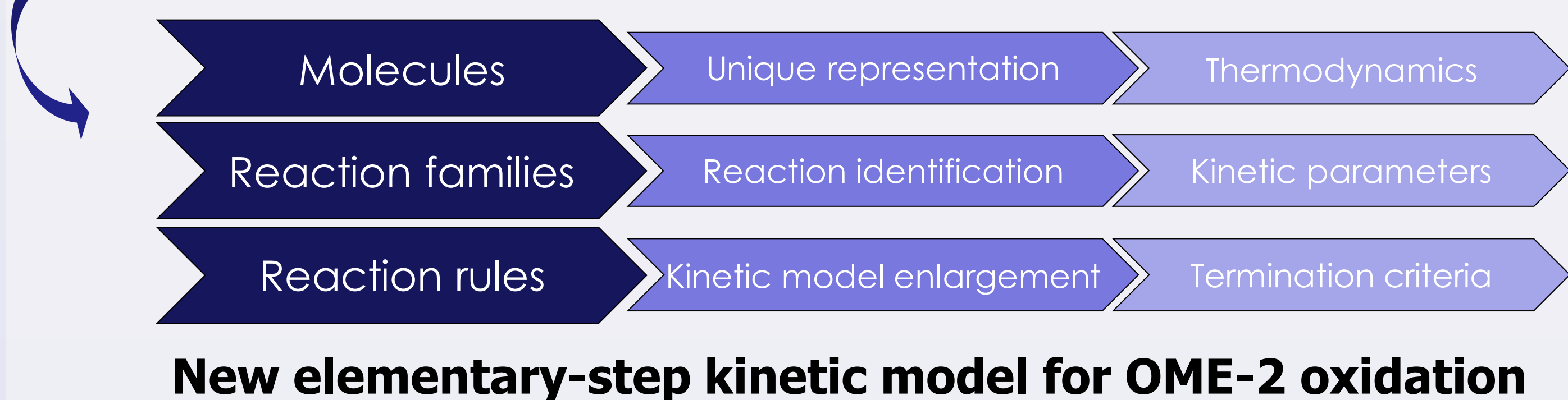
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Motivation

Oxymethylene ethers (OMEs) are a high-potential class of sustainable synthetic fuels when produced via **carbon capture** and **renewable electricity**. Their original backbone structure, composed of a **carbon-oxygen** atoms alternation, is promising for **soot reduction** in exhaust gases. A complete understanding of the **pyrolysis and combustion** mechanisms, covering the low- and high-temperature range, is a prerequisite to introduce OMEs as fuels on a large scale.

Modeling approach

- Quantum chemical calculations** at the CBS-QB3 level of theory for exploration of the Potential Energy Surface (PES) & determination of **thermodynamic** and **kinetic parameters** [1]
- Automatic **kinetic model** construction using the in-house developed tool **Genesys** based on hydrocarbons oxidation [2]

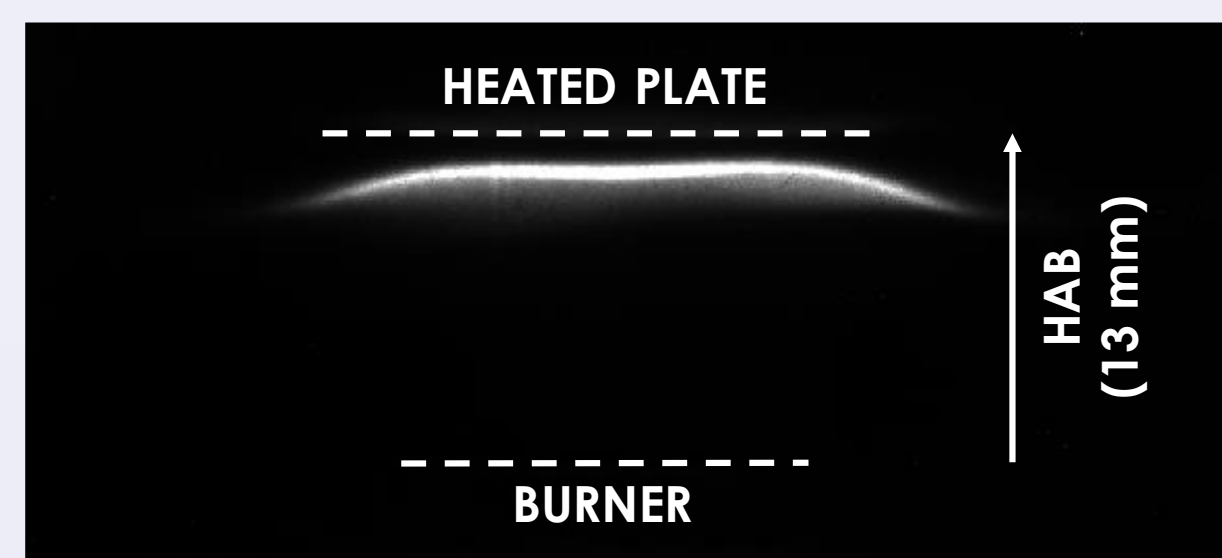


Low-temperature oxidation of oxymethylene ether-2 (OME-2)

*HAB = Height Above Burner

Experimental setup

- Stagnation plate burner: Allows the study of stabilized cool flames [3]
- Lean **OME-2/DME/O₂** cool flames stabilized with ozone
- Flame temperature: Type-K thermocouple, Ø = 250 µm
- Stable species measurement: GC/MS and online MS

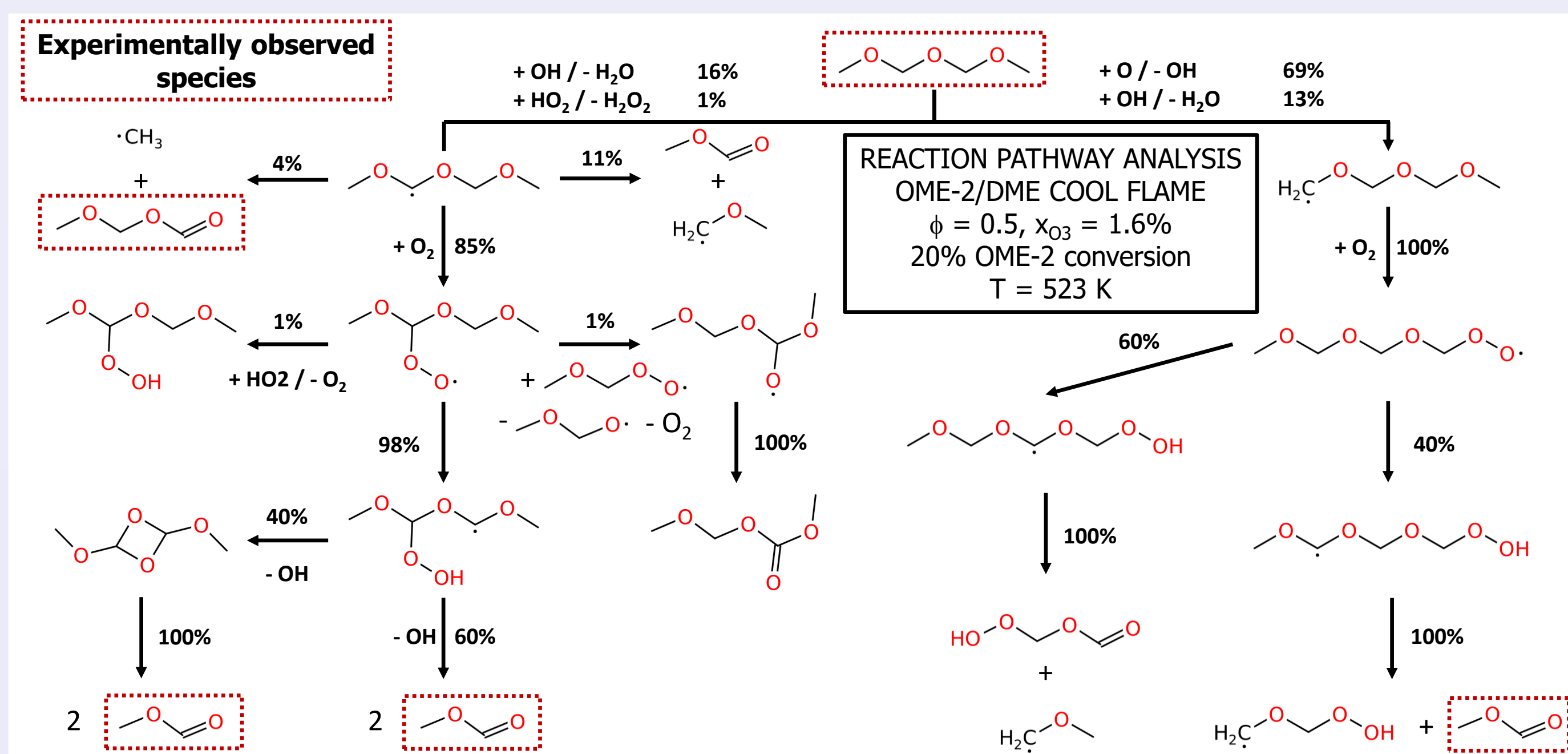
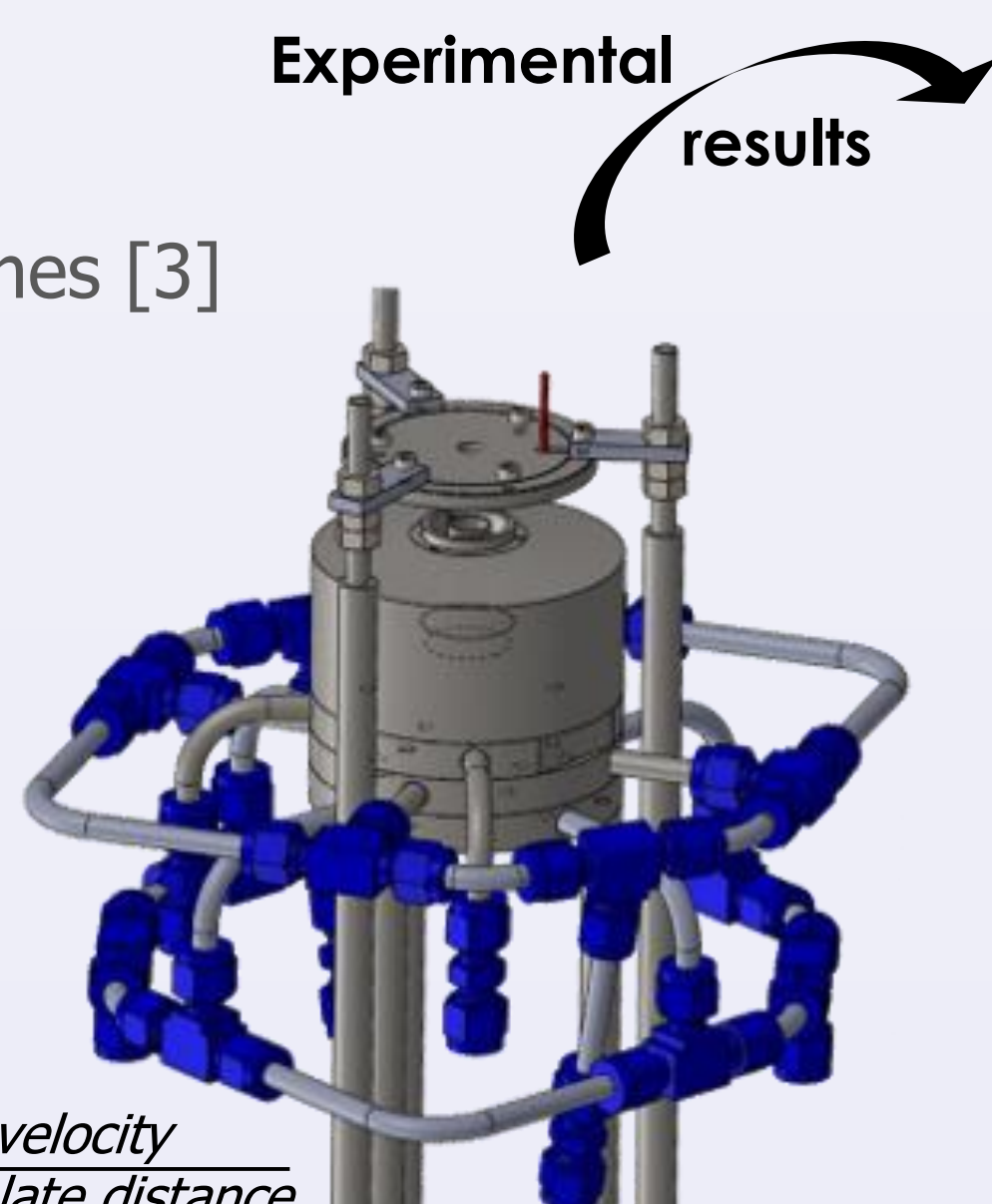


Raw chemiluminescence image (CH₂O*)

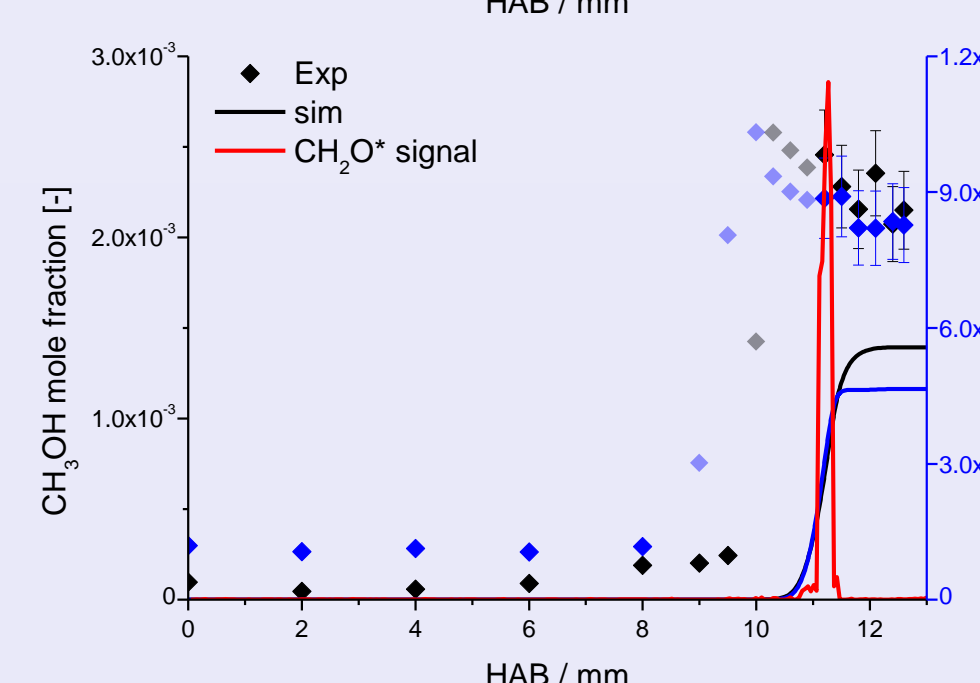
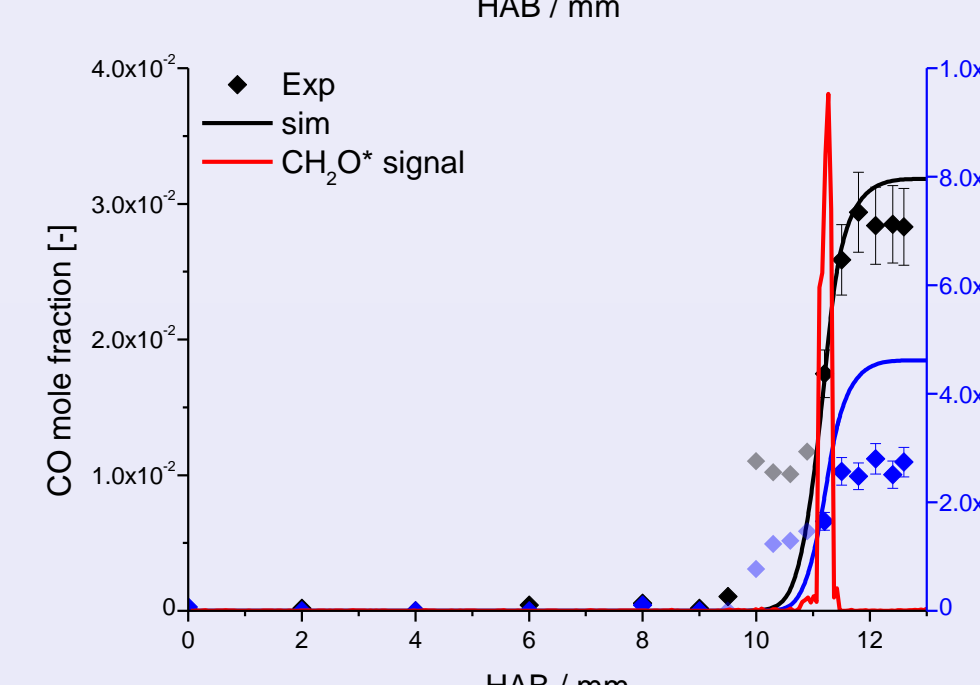
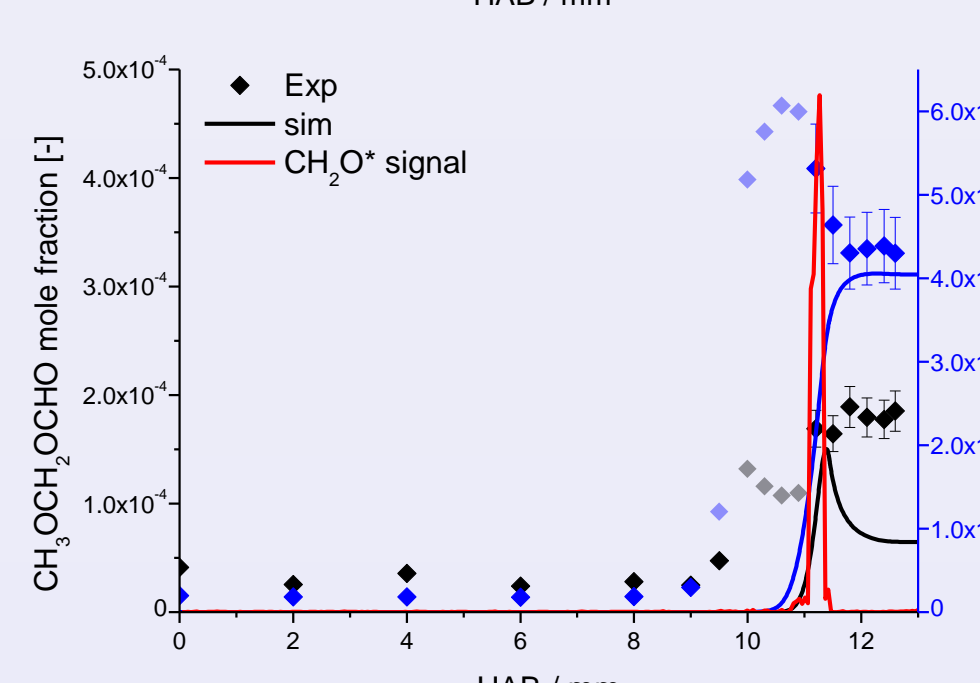
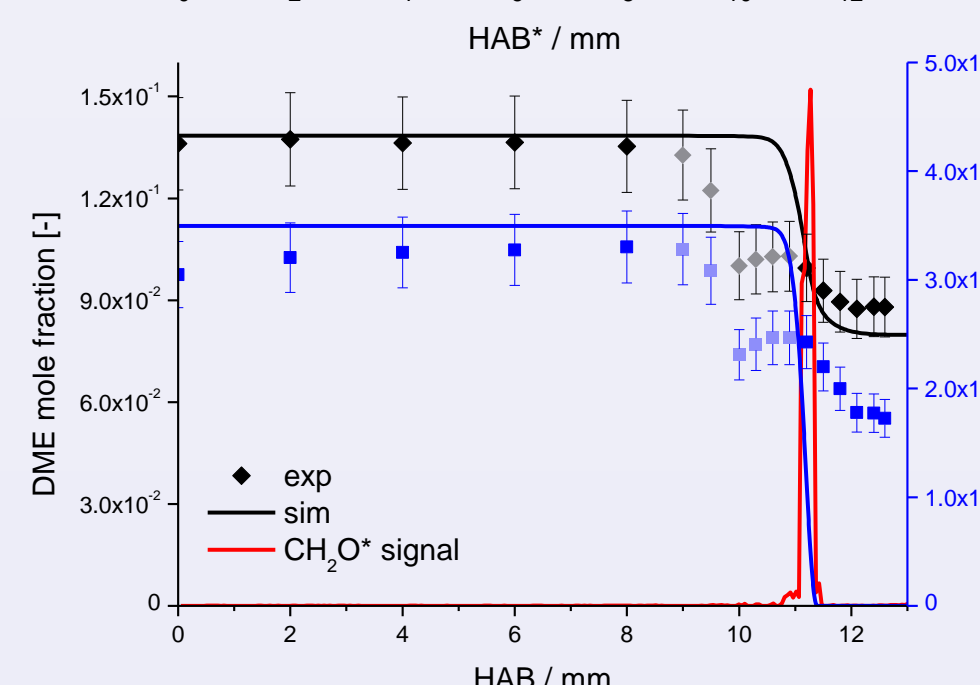
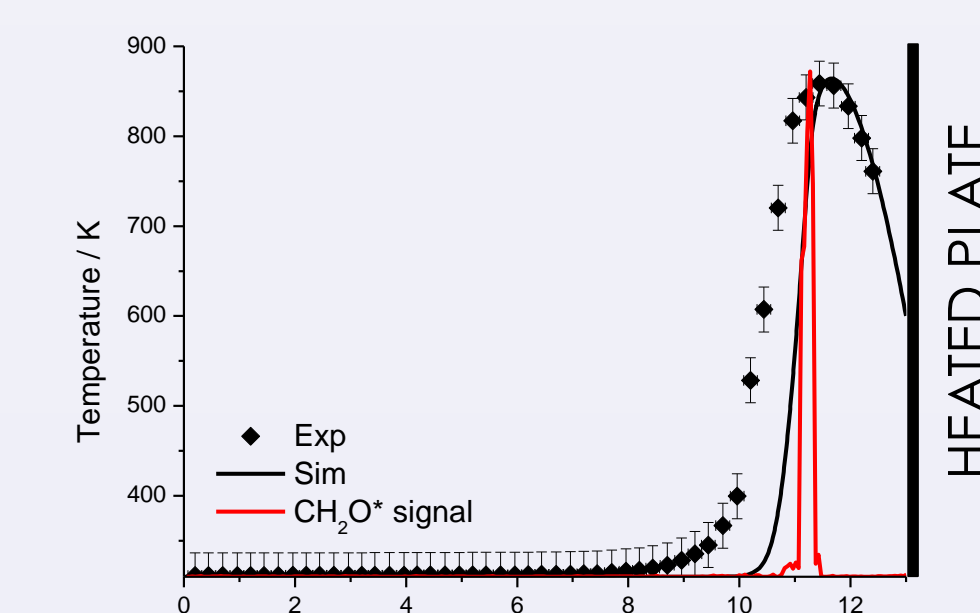
Cool flame characteristics

$\phi = 0.5$
 $\alpha^* = 50 \text{ s}^{-1}$
 $X_{O_3} = 1.6\%$
 2.5% OME-2/97.5% DME

$$\alpha^* = \frac{\text{gas velocity}}{\text{burner-plate distance}}$$



- H-abstraction** on the fuel molecule is mainly carried out by **Ö** atoms and **ÖH** radicals due to **O₃ addition**. H-abstraction by **Ö** atoms occurs preferentially on terminal carbons.
- Unimolecular decomposition** of OME-2 does not occur in such conditions.
- Decomposition after the fuel radical addition on O₂ mainly leads to the formation of **CH₃OCHO** (methyl formate) and **CH₃OCH₂OCHO** (methoxymethyl formate).



Mechanism construction

Base mechanism
AramcoMech 1.3 [4]
 +
 OME-2 mechanism (this work)
Genesys
 +
 O₃-submechanism
Foucher et al. [5]

- Excellent agreement of the model on the **flame temperature and position**.
- Partial conversion of the fuel** inside the cool flame → Typical of the low-temperature combustion regime.
- Early reactivity observed during the sampling experiments due to the presence of ozone in the sampling probe
 → **Does not impact** the species distribution after the cool flame.
- Methoxymethyl formate** (CH₃OCH₂OCHO) observed as the only OME-2 specific product in these conditions.
- Overestimation of the OME-2 conversion in the cool flame, but will be improved after including second QOOH addition on O₂ in the model.
- Fair agreement of the model on **oxygenated species** formed during the low-temperature oxidation of OME-2 and DME.
- High CO/CO₂ ratio** after the cool flame caused by the low temperature of the flame.
- Interactions** between O₃ and OME-2 not currently present in the developed model, could slightly shift the reactivity.

Conclusions & Work-in-progress

- A first principles based kinetic model for the low-temperature oxidation of oxymethylene ether-2 (OME-2) has been developed.
- The model was validated with novel data of a lean DME/OME-2 cool flame stabilized in a stagnation plate burner.
- Accounting for appropriate kinetics for the second QOOH addition on molecular oxygen leading to the formation of ketohydroperoxides and newly calculated reaction rate coefficients of hydrogen abstraction by ozone and atomic oxygen are expected to improve the model performance.

References

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