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Experimental and modeling study of the high-temperature combustion chemistry of tetrahydrofurfuryl alcohol

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Energy demand of the transport sector

~ 25%-50%

increase in energy demand by transport sector by 2040

[ExxonMobil 2019]

~ 90%

of today's liquid fuels are made from **petroleum**

[ExxonMobil 2019]

- Problem of pollutant emissions
- Greenhouse gas emissions
- Depletion of reserves
- Increase of costs

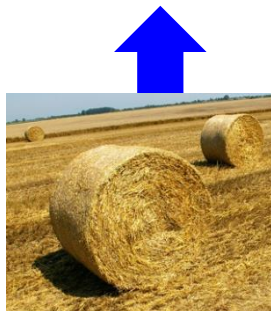


Interest of biofuels

Advanced biofuels

(second and third generations)

- Renewable energy source
- Decrease of dependance on petroleum
- Energy security
- Already mature production methods
- Many applications already developed

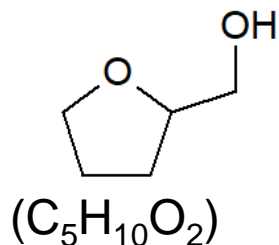


Cellulosic biomass



Micro-algae

THFA: promising biofuel



THFA

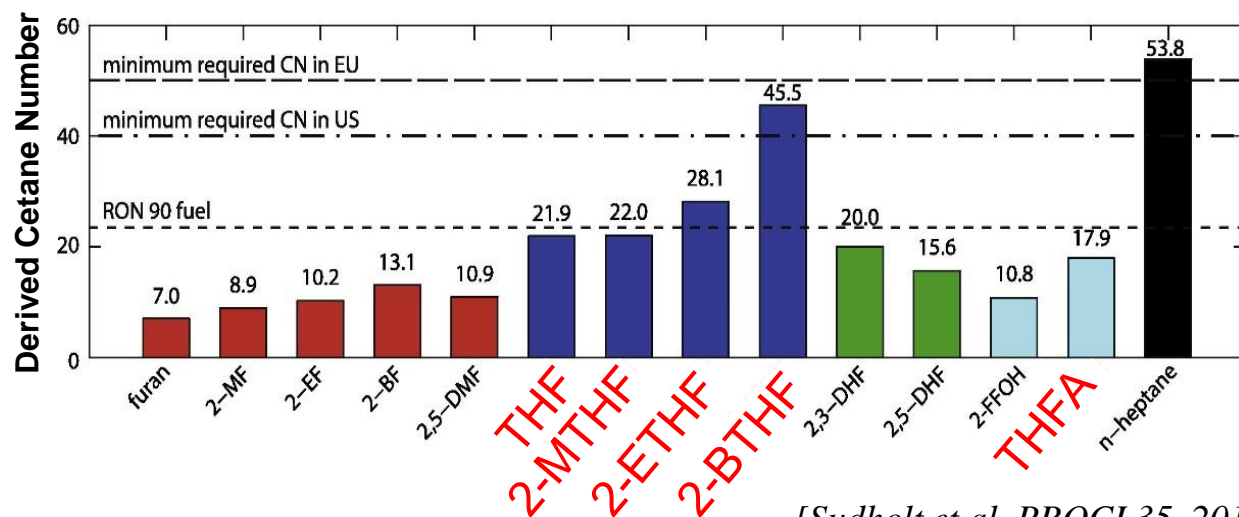
(TetraHydroFurfuryl Alcohol)



Boiling Point:
178 °C (gasoline: 30-200)

Lower Heating Value:
27.5 MJ/L (ethanol: 21.3)

Suitable as a fuel additives for gasoline engines

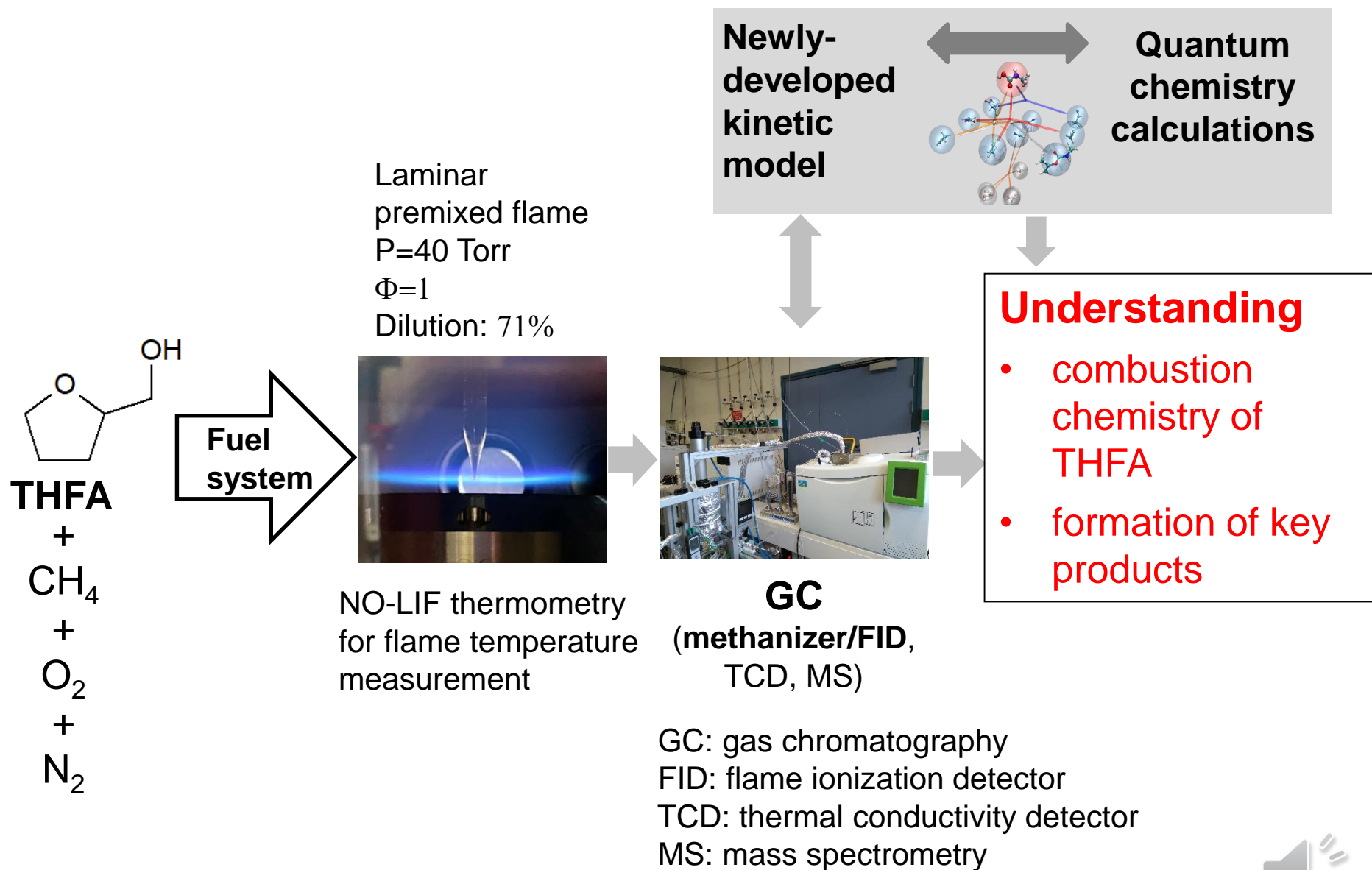


[Sudholt et al. PROCI 35, 2015]

- Studies on production, spray propagation, ignition are known.
- Combustion chemistry and species profiles have not yet been reported



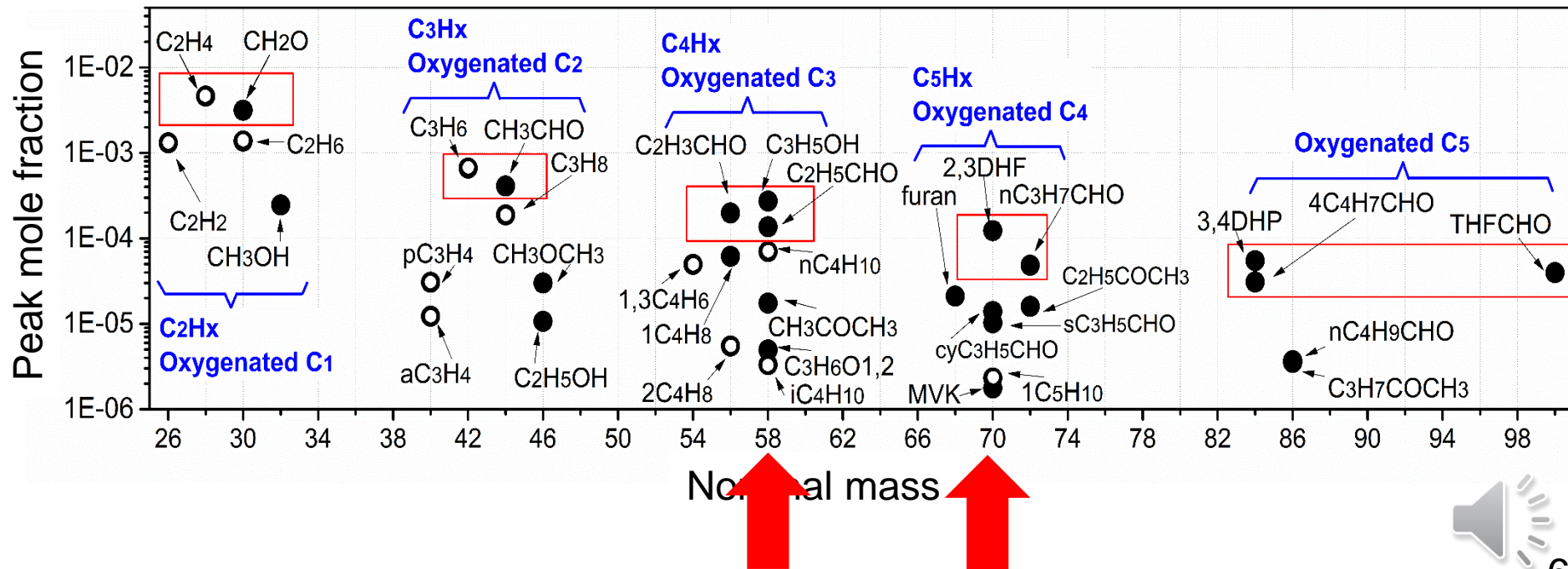
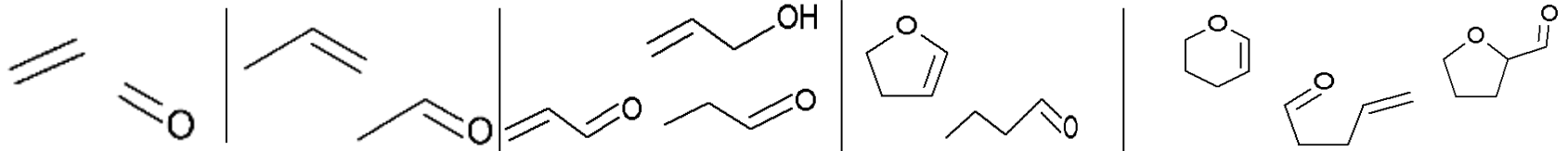
THFA: flame chemistry in the present study



Experimental results

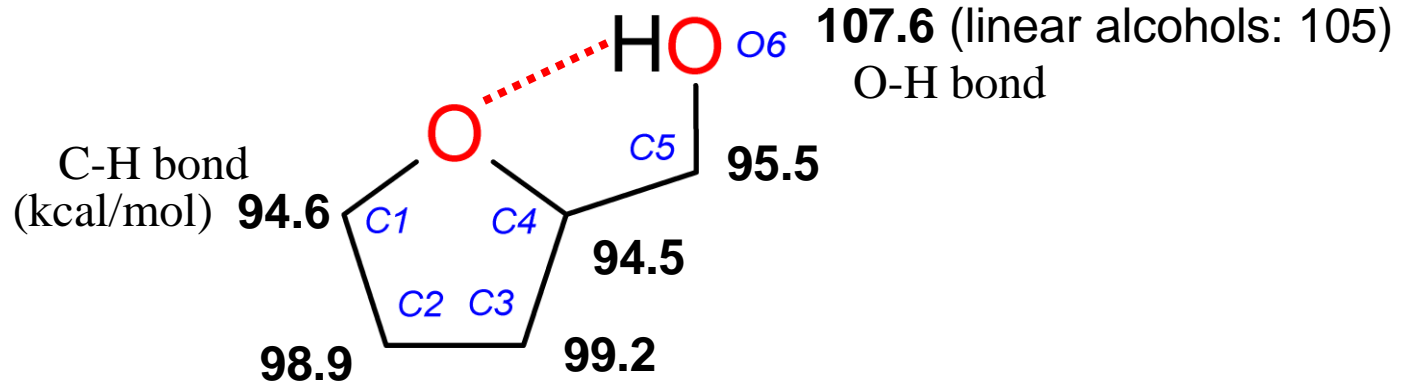
43 quantified species: fuels + final products + 35 intermediate species

- Highly complex compositions, e.g. $m/z=58$ (6 species), $m/z=70$ (5 species)
- Crucial for knowing the nature of pollutants, analyzing the reaction mechanism.

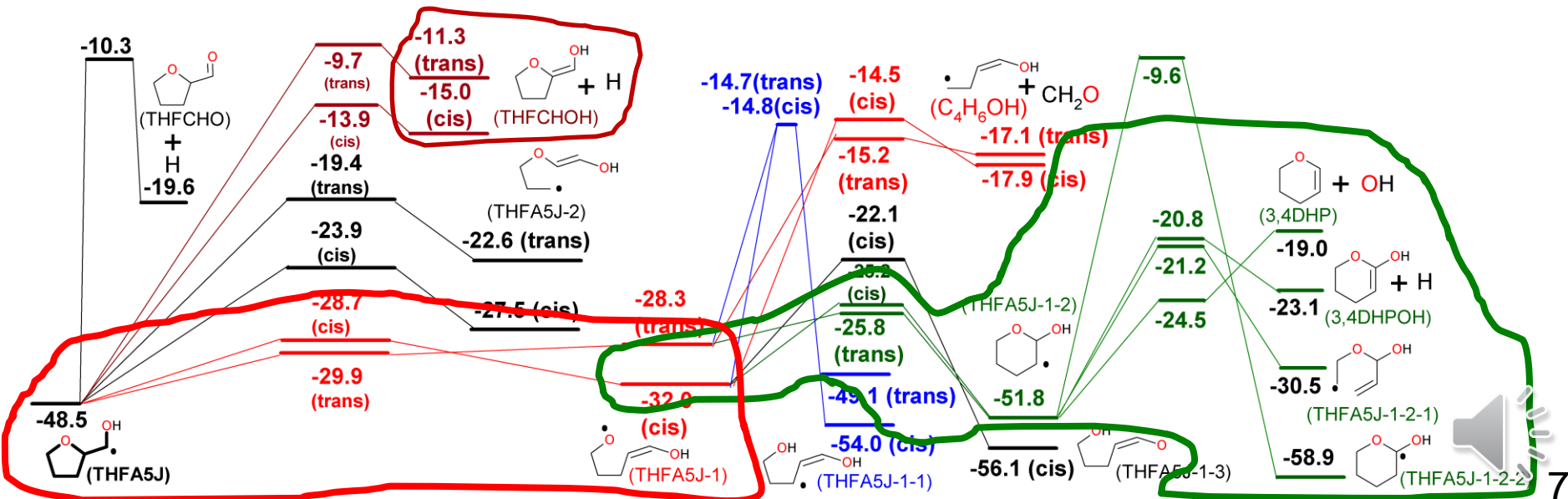


Model development

THFA reaction subset: rely upon theoretical calculations (CBS-QB3)



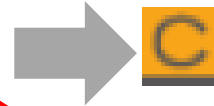
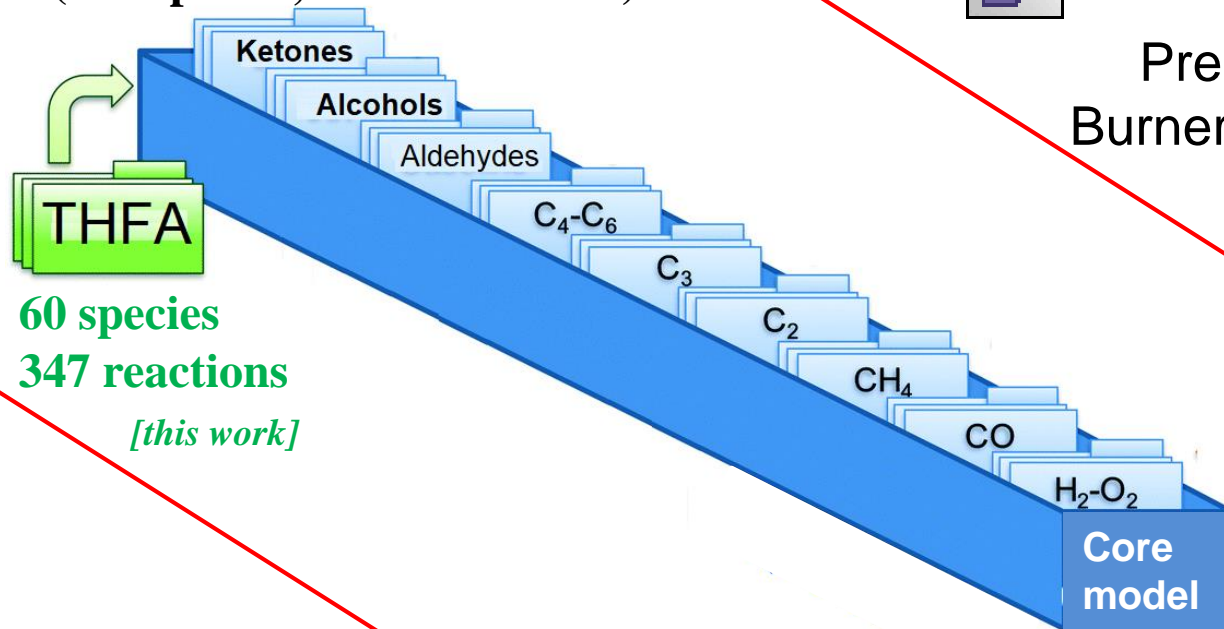
- Potential Energy Surface was examined for important fuel radicals
 - +CIS is more stable than TRANS
 - +Low energy barrier of C-O beta scission
 - +Importance of ring enlargement chemistry established



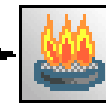
Model development

First detailed kinetic model for HT combustion of THFA

Detailed kinetic model
for THFA combustion
(479 species, 2914 reactions)



ANSYS Chemkin-Pro 2019 R1



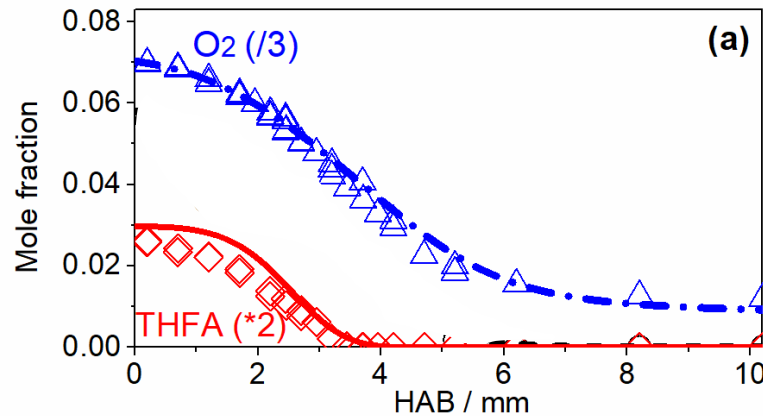
Premixed Laminar
Burner-Stabilized Flame

[De Bruycker et al.
CnF 176, 2017]

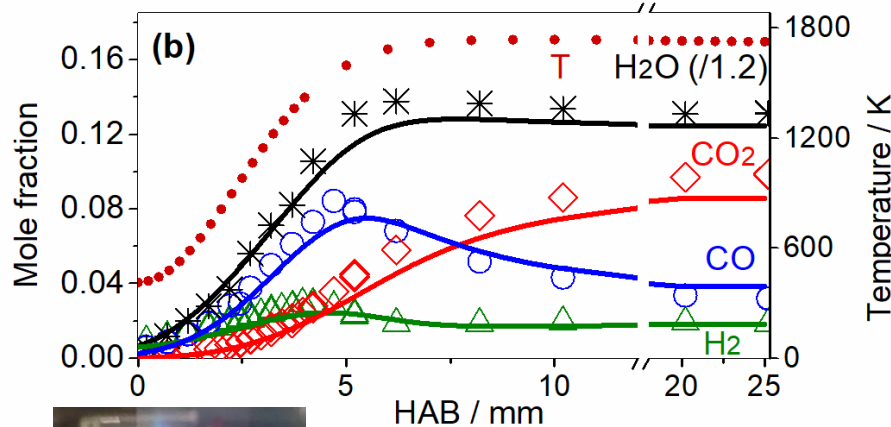


Comparison of model and experiment

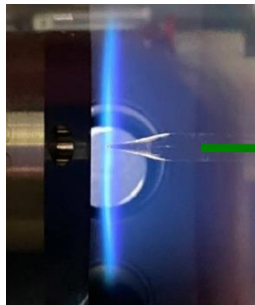
Excellent agreement between model predictions and experiments for fuel consumption and final products. Experimental T-profile used as input.



Symbols: experiment
Lines: present model



Temperature (T) profile by
NO-LIF and Thermocouple



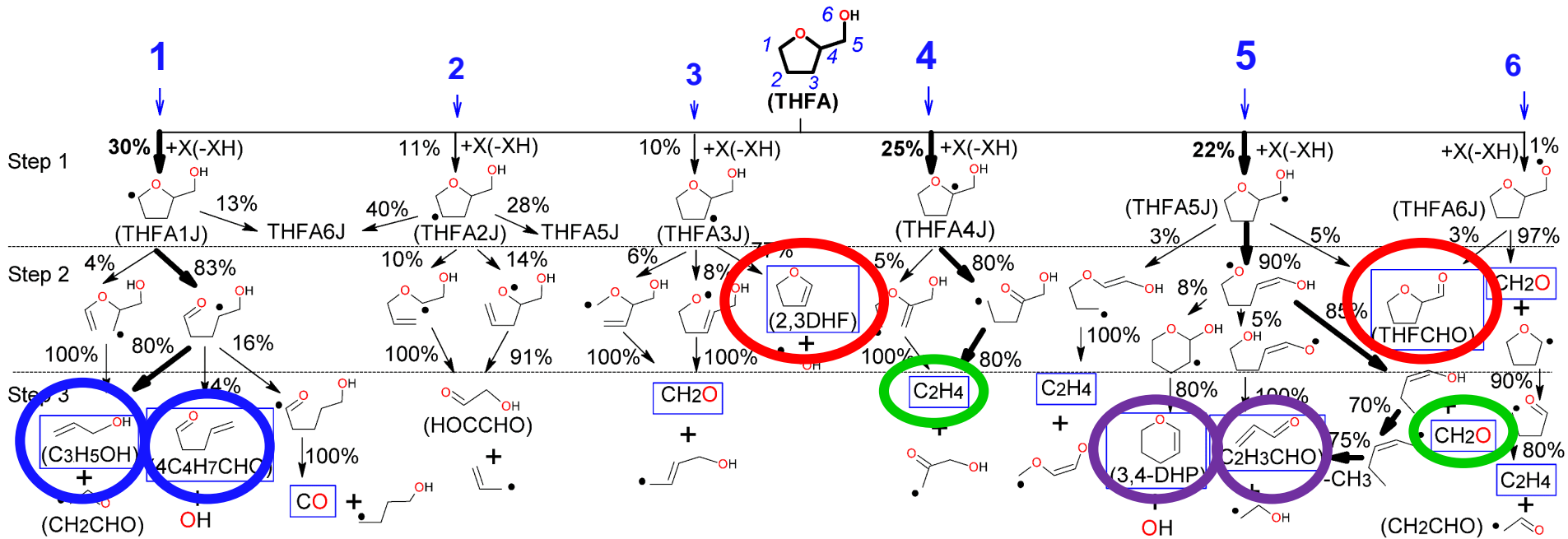
HAB: Height Above the Burner



Comparison of model and experiment

Reaction path analysis on THFA consumption and intermediate formation

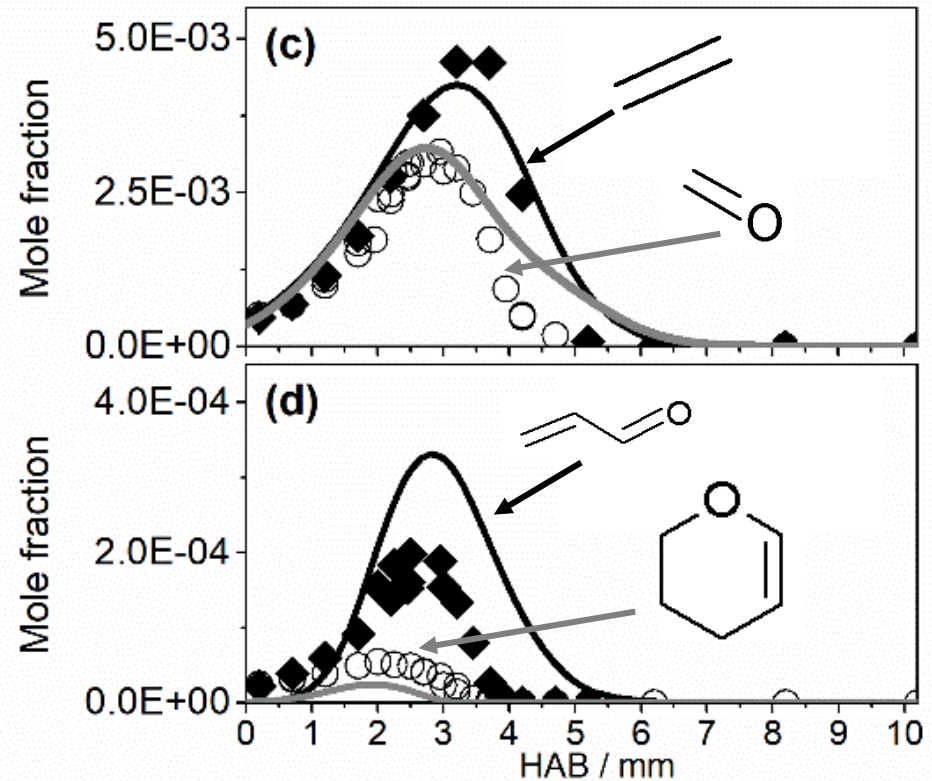
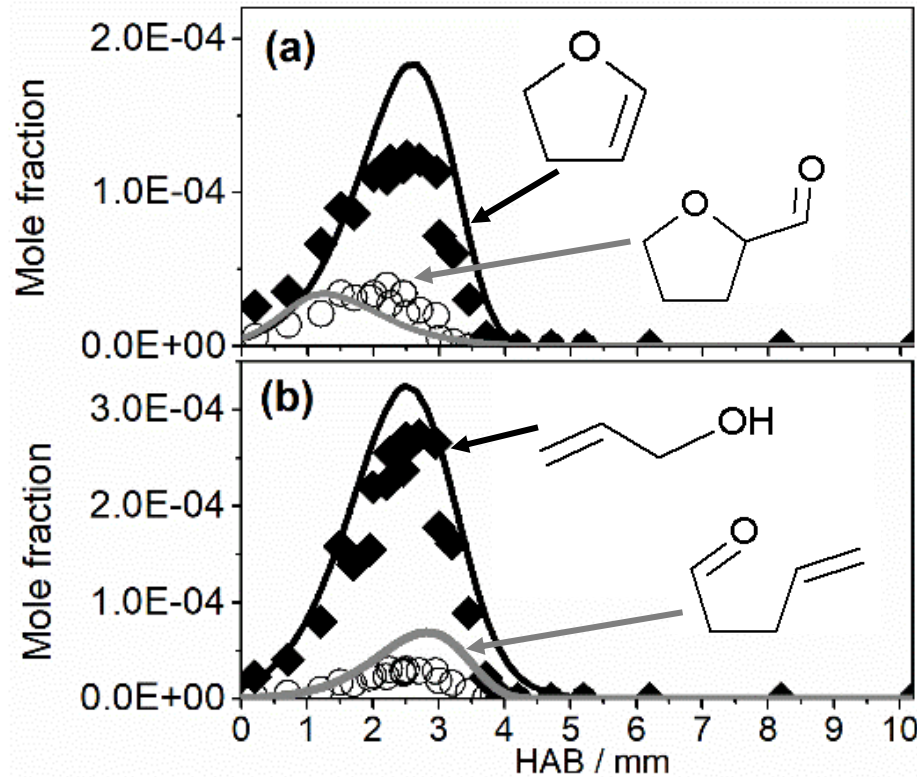
- Significant THFA consumption paths: **1, 4, 5**
- Most of important species were detected in experiments



Comparison of model and experiment

Quite good agreement between model predictions and experiments for intermediate profiles

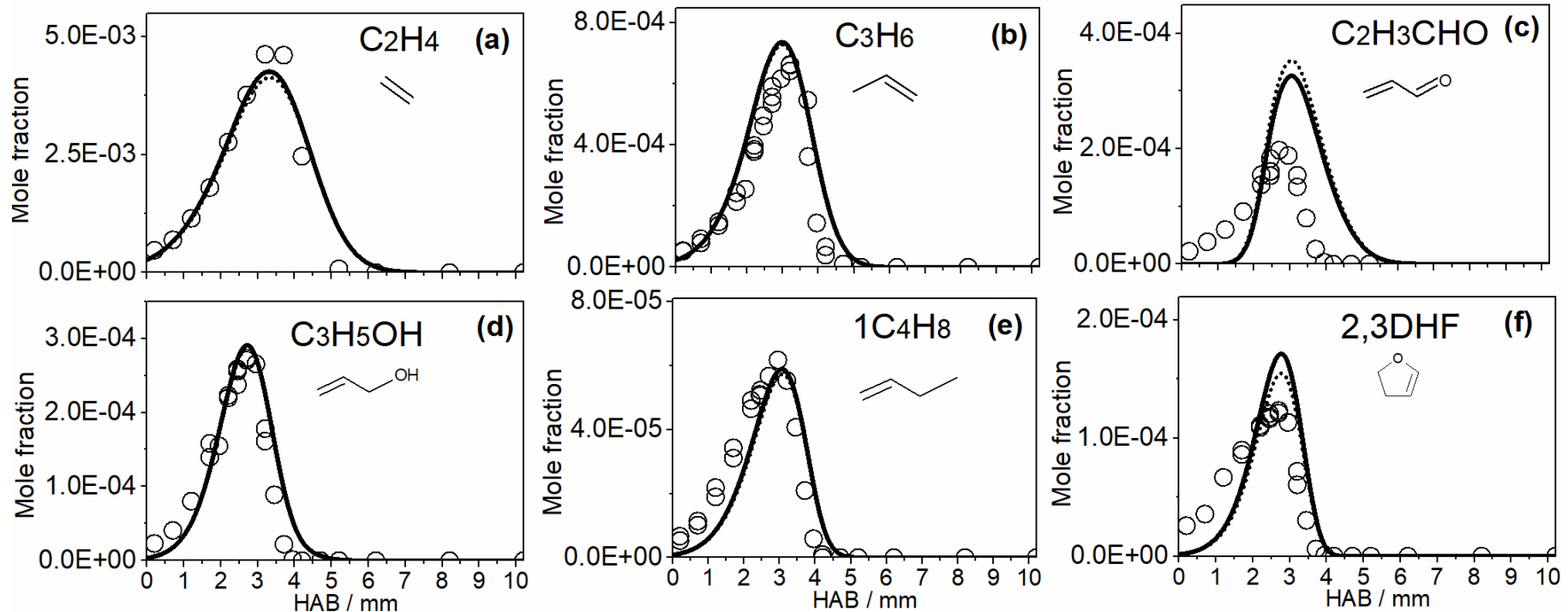
Symbols: experiment
Lines: present model



Comparison of model and experiment

CIS or TRANS of species in THFA sub-model: only insignificant changes in the predictions

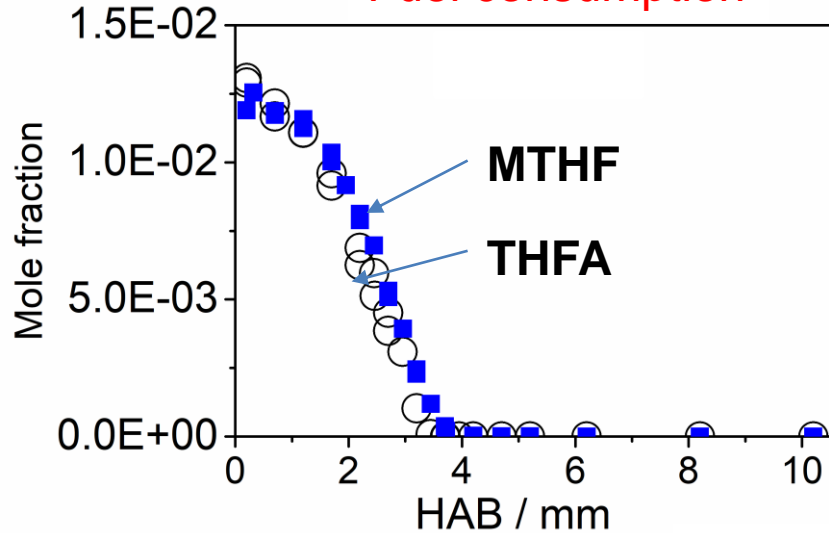
Solid lines: present model with CIS configuration (thermo + rate coefficients)
Dashed lines: present model with TRANS configuration



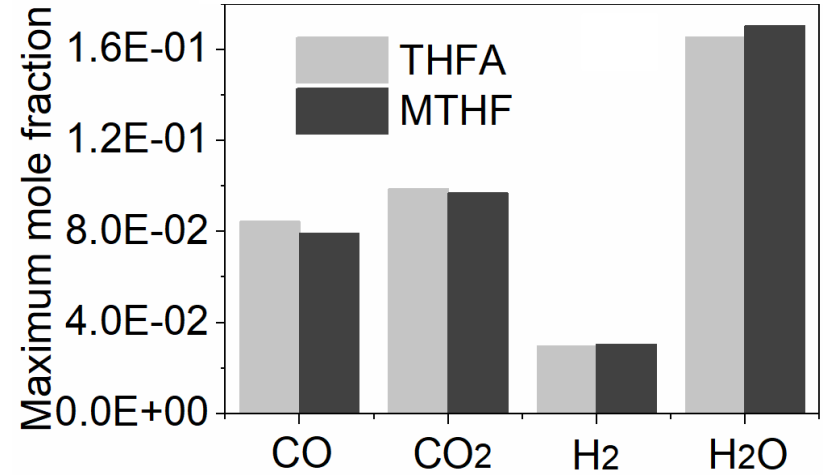
Ongoing study

Comparison: **THFA** OC1CCOC1 vs. **MTHF** CC1CCOC1

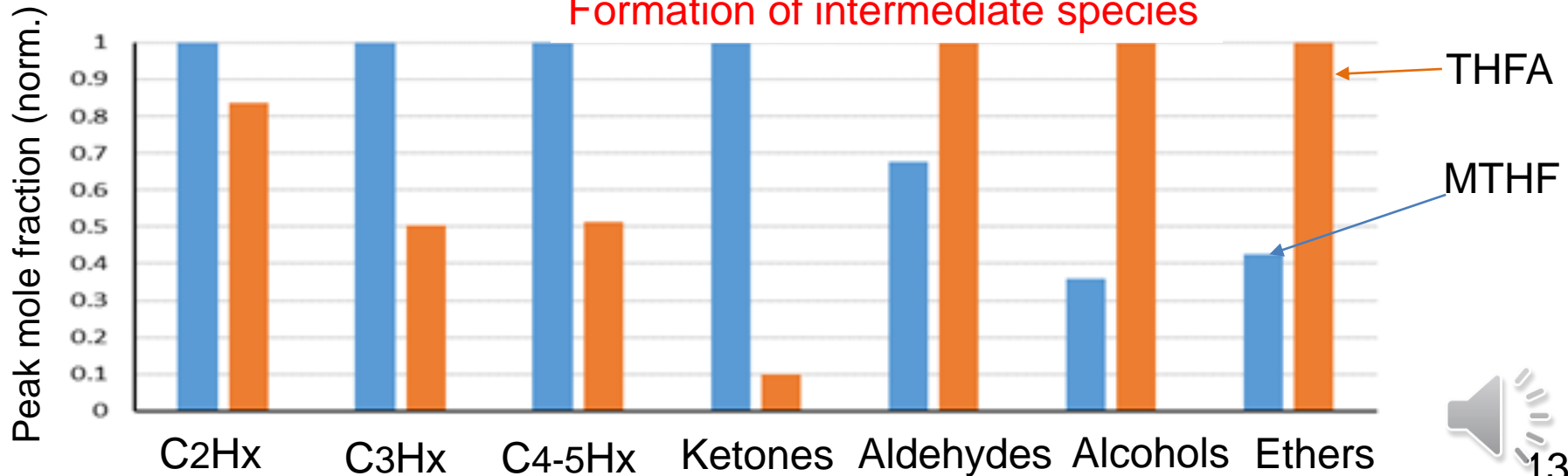
Fuel consumption



Formation of major products



Formation of intermediate species



Thank you for attention

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