Development of a comprehensive plasma-chemical kinetic mechanism for low-temperature oxidation of undiluted H_2/O_2 mixtures

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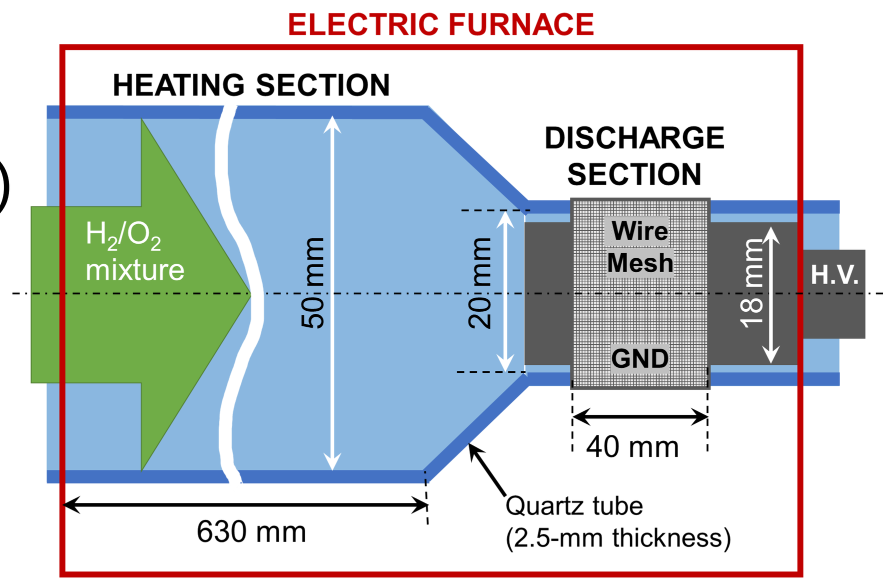
Introduction

In the quest for more efficient and cleaner combustion and fuel reforming technologies, a (renewed) interest has been sparked in non-equilibrium plasma discharges [1].
Important early studies lacked experimental data for validation at temperatures below 800 K, while most recent work either focuses on highly diluted and/or sub-atmospheric conditions. However, due to the complexity of plasma assisted systems, the translation of these studies to different (more realistic) conditions is limited [2].
Therefore, it is essential to develop a temperature-dependent plasma-chemical reaction mechanism validated by experimental data below 1000 K, suitable to study temperature-dependent plasma assisted processes [1].

Methodology

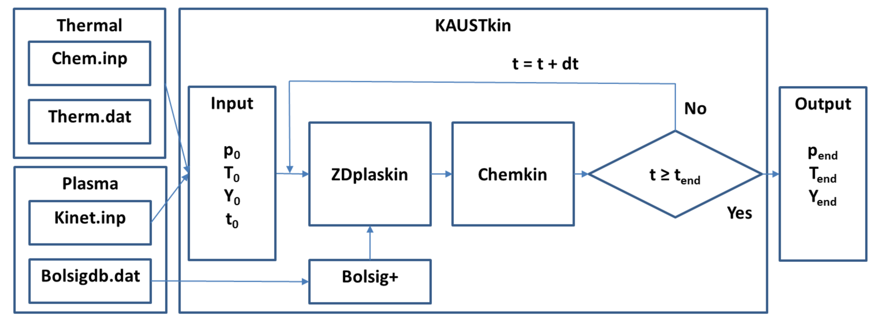
Experimental set-up

- Temperature-controlled DBD
- H_2/O_2 mixture (ϕ = 0.01–49.5)
- Flow = 200 sccm
- P_{dis} = 1.25–20 W
- GC and FTIR analysis



Modelling set-up

- KAUSTKin [2]
- Plasma-chemical mechanism:
  - Adjusted NUIGMech1.1
  - Plasma H_2/O_2
  - O_3 reactions



Acknowledgements

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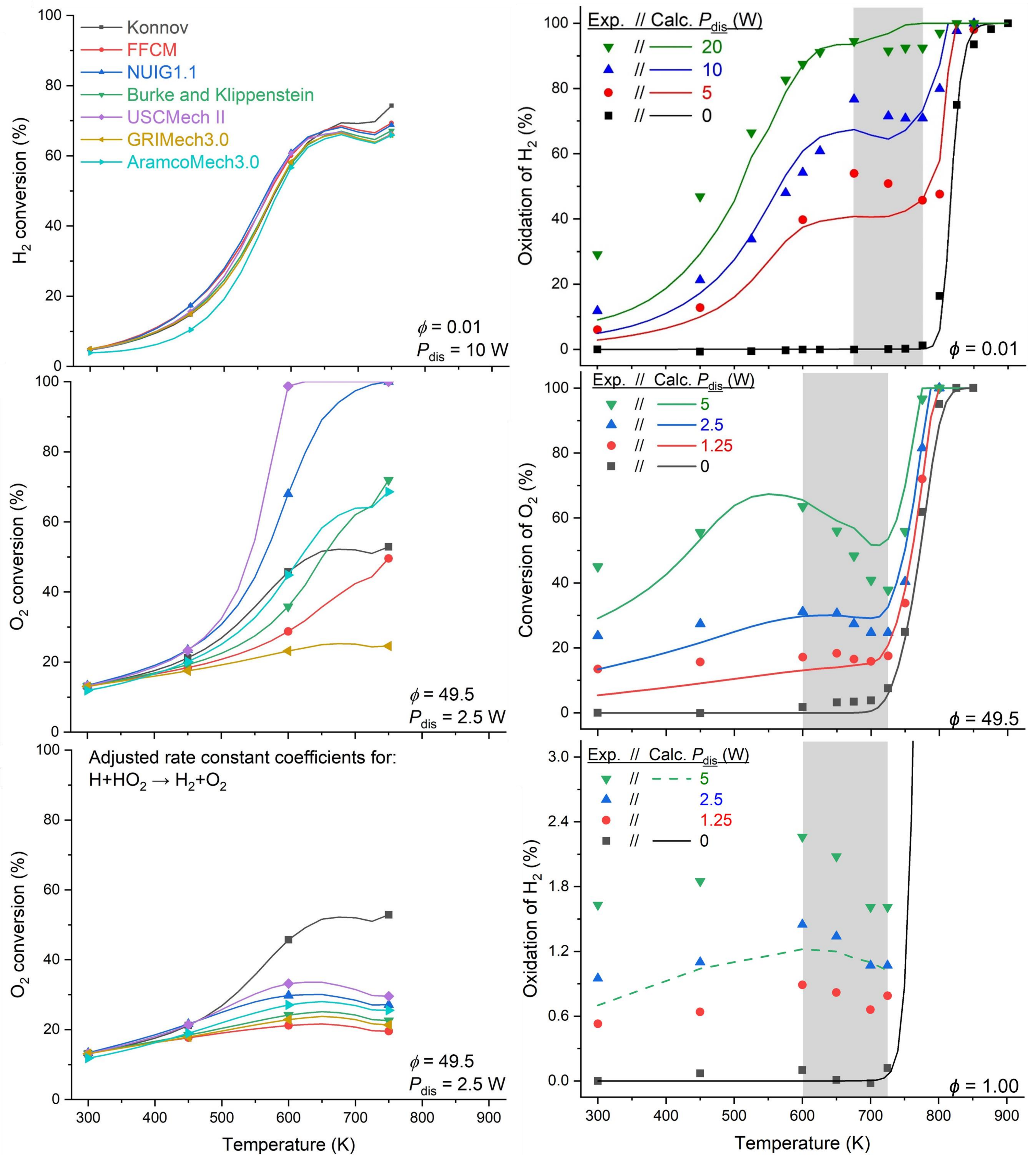
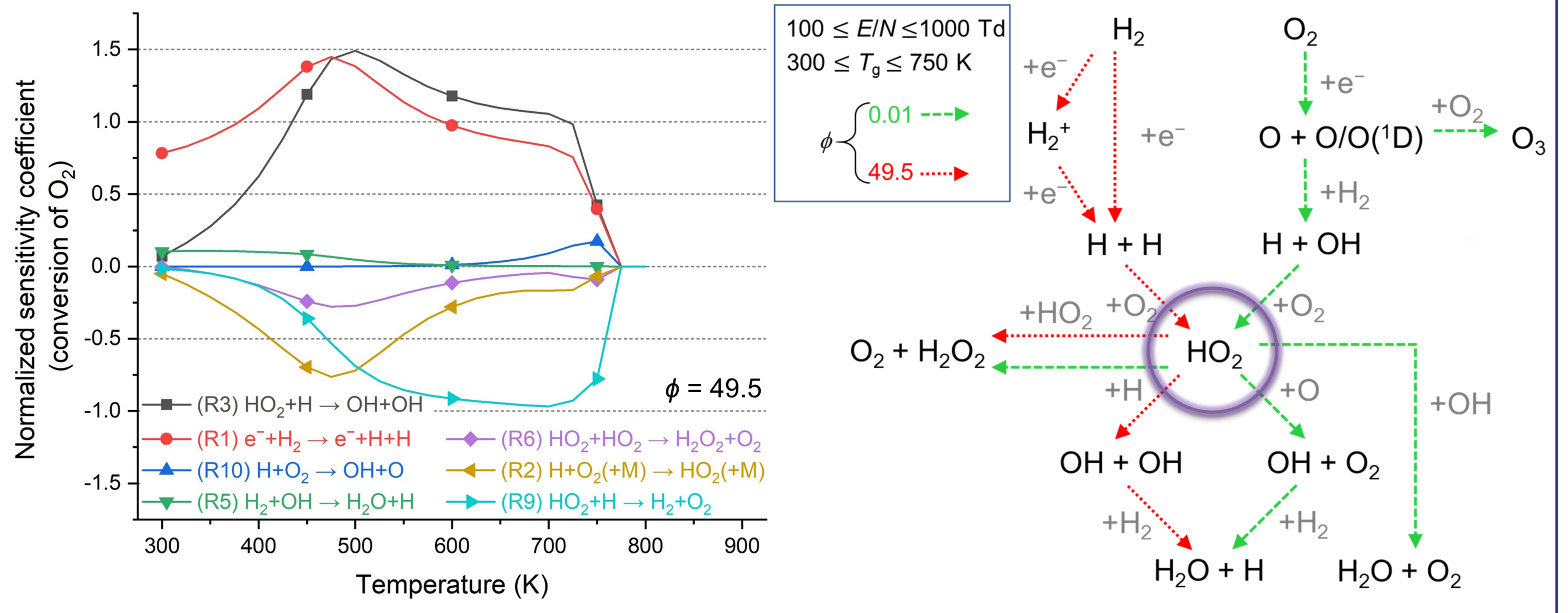
Results

Mechanism comparison and validation



Kinetic analysis



Summary

Plasma-chemical kinetics:
- High sensitivity for H and HO_2 reactions
- HO_2 key oxidation intermediate

NTC-like behavior [2,3]:
- Physical effect of *E/N*
- Chain branching ↔ termination

Ongoing Work

- Further modification of the HO_2 chemistry to improve the mechanism performance for (near) stoichiometric mixtures:
  1) Rate adjustments based on known uncertainties
  2) Addition of missing HO_2 interactions with H_2O_2
- Addition of N_2 chemistry and addition of hydrocarbons
- Use as chemical kinetic tool to improve reaction mechanisms

References

[1] M.S. Cha and R. Snoeckx, *Front. Mech. Eng.*, **2022**, *8*, 1–5
[2] R. Snoeckx et al., *Combust. Flame*, **2022**, *242*, 112205
[3] R. Snoeckx and M.S. Cha, *in preparation for Combust. Flame*