

Technical University of Denmark



Propane Oxidation at High Pressure and Intermediate Temperatures

Hashemi, Hamid; Christensen, Jakob Munkholt; Glarborg, Peter

Publication date:
2016

Document Version
Peer reviewed version

[Link back to DTU Orbit](#)

Citation (APA):

Hashemi, H., Christensen, J. M., & Glarborg, P. (2016). Propane Oxidation at High Pressure and Intermediate Temperatures. Poster session presented at 36th International Symposium on Combustion, Seoul, Korea, Republic of.

DTU Library

Technical Information Center of Denmark

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Propane Oxidation at High Pressure and Intermediate Temperatures

Hamid Hashemi, Jakob M. Christensen, Peter Glarborg

Department of Chemical Engineering, Technical University of Denmark (DTU), DK-2800 Kgs. Lyngby, Denmark

Email: pgl@kt.dtu.dk (P. Glarborg)

hah@kt.dtu.dk (H. Hashemi)



Experimental: Laminar Flow Reactor (FR)

- ❖ Quartz reactor to minimize surface reactions
- ❖ Steel pressure shell to achieve high pressures
- ❖ Temperature: 500–900 K
- ❖ Pressure: 100 bar
- ❖ Isothermal Zone Length: 42–44 cm
- ❖ Residence time: 8–11 s
- ❖ Measurement via GC and Gas Analyzer

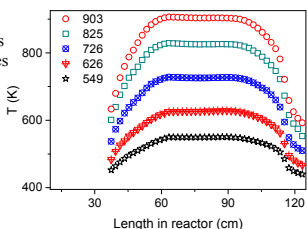


Fig 1. Temperature profile measured inside the pressure-shell wall of the reactor

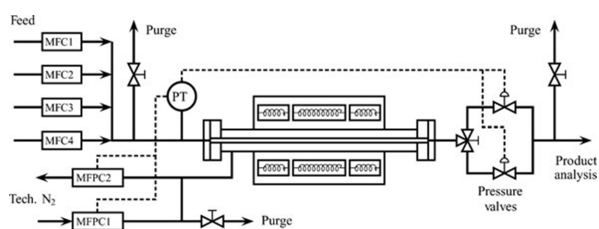


Fig 2. Schematic diagram of the high pressure laminar flow reactor

Chemical Kinetics Model

- ❖ H₂/CO/HC's subsets from recent work by Glarborg et al. [1–3].
- ❖ C₃ subset is reviewed and introduced in *p.w.*
- ❖ Low temperature sequences for propane oxidation is adopted from Goldsmith et al. [4].

Results: Flow Reactor (FR)

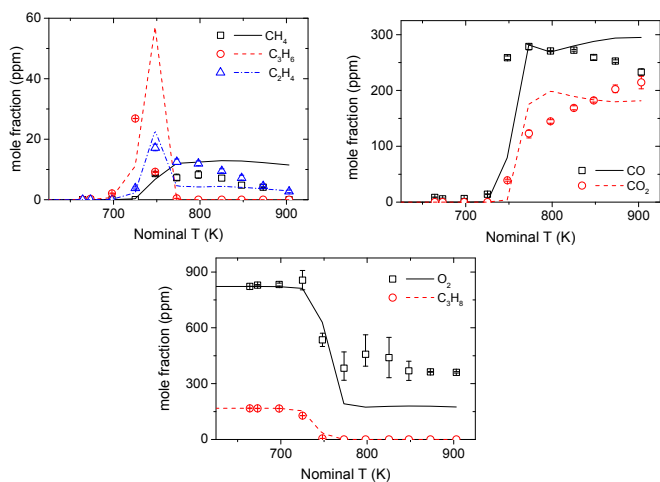


Fig 3. Experiments in the flow reactor at 100 bar pressure. The initial conditions were 168/ 822 ppm of C₃H₈/O₂ in N₂ (Φ=1). Residence time varies between 8 and 11 s.

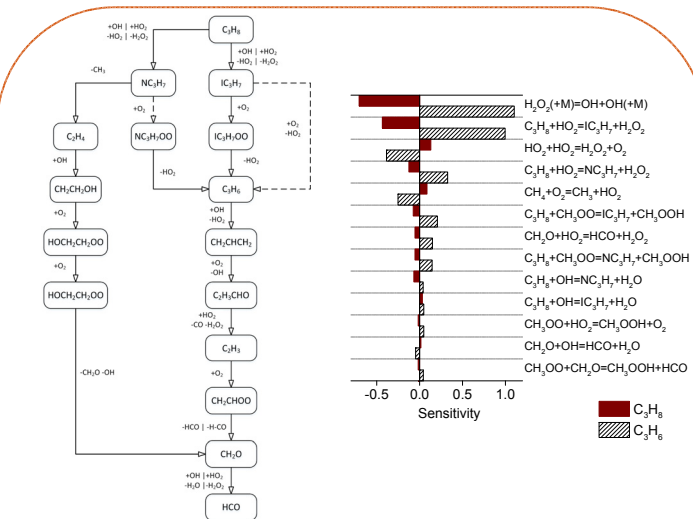


Fig 4. Left: Reaction pathways of propane oxidation at conditions investigated in the flow reactor (100 bar, 750 K). Right: Sensitivity of C₃H₈ and C₃H₆ prediction under flow-reactor conditions (100 bar, 750 K).

Results: Comparing the Model with Literature

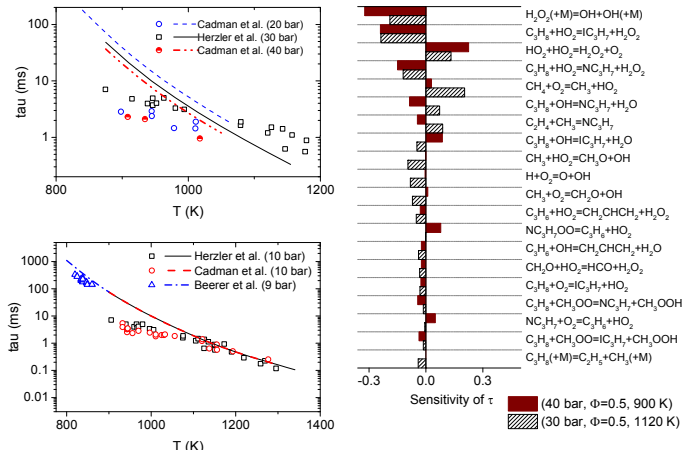


Fig 5. Left: Ignition delay times of propane. The experiments are from Herzler et al. [5] and Cadman et al. [6] (2.1% C₃H₈ + 20.6% O₂ in N₂, Φ=0.5), and Beerer et al. [7] (2.5% C₃H₈ + 20.5% O₂ in N₂, Φ=0.6). Right: Sensitivity of ignition delay time of propane to reaction rate constants (2.1% C₃H₈ + 20.6% O₂ in N₂, Φ=0.5).

Summary & Future Work

- ❖ Propane oxidation in the flow reactor:
 - Onset at 725–750 K (100 bar, Φ=1)
 - Accurate model prediction
 - Importance of abstraction reaction C₃H₈+ HO₂
- ❖ The model prediction of ignition delay times:
 - Over-prediction at intermediate T (900–1000 K)
 - Inaccuracy in transition from low-T to high-T regimes
- ❖ Further experiments on propane oxidation at different P and Φ are planned.
- ❖ Further work is required to improve the model prediction, especially for ignition delays.

References

- [1] H. Hashemi, J. M. Christensen, S. Gersen, P. Glarborg, "Hydrogen oxidation at high pressure and intermediate temperatures: Experiments and kinetic modeling", Proc. Combust. Inst. 35 (2015) 553–560.
- [2] H. Hashemi, J. M. Christensen, S. Gersen, H.B. Levinsky, S.J. Klippenstein, P. Glarborg, "High-pressure oxidation of methane", Combust. Flame (accepted), 2016.
- [3] J. Lopez, C. Rasmussen, H. Hashemi, M. Alzueta, Y. Gao, P. Marshall, C. Goldsmith, P. Glarborg, "Experimental and kinetic modeling study of C₂H₂ oxidation at high pressure", Int. J. Chem. Kinet. (accepted), 2016.
- [4] C. F. Goldsmith, W. H. Green, S. J. Klippenstein, "Role of O₂ + QOOH in low-temperature ignition of propane. 1. Temperature and pressure dependent rate coefficients", J. Phys. Chem. A 116 (2012) 3325–3346.
- [5] J. Herzler, L. Jerig, P. Roth, "Shock-tube study of the ignition of propane at intermediate temperatures and high pressures", Combust. Sci. Technol. 176 (2004) 1627–1637.
- [6] P. Cadman, G. O. Thomas, P. Butler, "The auto-ignition of propane at intermediate temperatures and high pressures", Phys. Chem. Chem. Phys. 2 (2000) 5411–5419.
- [7] D. Beerer, V. McDonell, S. Samuelsen, L. Angello, "An experimental ignition delay study of alkane mixtures in turbulent flows at elevated pressures and intermediate temperatures", J. Eng. Gas Turbines Power 133 (2011) 011510.