Propane Oxidation at High Pressure and Intermediate Temperatures

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

Publication date: 2017

Document Version: Peer reviewed version

Citation (APA):

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)

Motivations

- Propane: a major component in LPG
- Propane: a minor but sensitive component of natural gas
- Engines and gas turbines: need experimental data at high pressures and intermediate temperatures

Experimental: laminar flow reactor

- Quartz reactor to minimize surface reactions
- Steel pressure shell to achieve high pressures
- Pressure: 100 bar
- Isothermal Zone Length: 42—44 cm
- Residence time: 5—11 s
- Measurement via GC

Chemical kinetics model

- H2/CO/HC’s subsets from recent work by Glarborg et al. [1—4].
- C3 subset is reviewed and introduced in the present work.
- Low temperature sequences for propane oxidation is adopted from Goldsmith et al. [5].

Results: fuel-rich mixture

Propane concentration dropped sharply at T=680 K for a fuel-lean mixture (oxidizing conditions), and propane vanished from the exhaust at T=725 K. The model predicted slower reactivity compared to the experiments, so the fuel conversion was slightly underpredicted by the model.

Results: stoichiometric mixture

For a stoichiometric mixture, the fuel conversion started around 725 K. At T>750 K, propane was consumed almost completely. The major products of the oxidation were CO and CO2 and the concentration of propene and ethene decreased sharply at T>775 K. The model captured the onset temperature of ignition accurately but it seems that CO oxidation to CO2 at high temperatures was not precisely captured by the model.

Summary

Propane oxidation at intermediate temperatures (500—900 K) and high pressure (100 bar) has been characterized by conducting experiments in a laminar flow reactor over a wide range of stoichiometries. The onset of fuel oxidation was found to be 600—725 K, depending on mixture stoichiometry. The model agreed well with the measurements of fuel-lean and stoichiometric mixtures while the model underpredicted the fuel conversion for fuel-lean conditions. Sensitivity analyses revealed the importance of H-abstraction reactions by HO2, OH, and CH3OO in controlling propane oxidation at 750 K.

References


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

Fig 3. Results of experiments under stoichiometric conditions (121 ppm C3H8 and 547 ppm O2 in N2, Φ=12.5) at 100 bar pressure.

Fig 4. Results of experiments under stoichiometric conditions (121 ppm C3H8 and 547 ppm O2 in N2, Φ=1-3) at 100 bar pressure.

Fig 5. Results of experiments under oxidizing conditions (146 ppm C3H8 and 3.405% O2 in N2, Φ=0.02) at 100 bar pressure.

Fig 6. Left: Reaction pathways for propane oxidation under stoichiometric conditions (750 K, 100 bar). Right: Sensitivity of C3H8 prediction under flow reactor conditions (RD: reducing, ST: stoichiometric, OX: oxidizing conditions) at 100 bar. The component HOOCH2CH2CH2OO is named “well_1” in above.

According to the results of sensitivity analyses, propane oxidation is largely controlled by H-abstraction by HO2 from propane (R1). The branch leading to iC3H7 shows a larger sensitivity compared to the other one (except for oxidizing conditions). The reaction between C3H8 and OH (R2) is also sensitive. While the branch to nC3H7 promotes the oxidation, the other branch to iC3H7 inhibits the fuel conversion. The H-abstraction by CH3OO from propane (R3) is also sensitive for reducing and stoichiometric conditions.

Analysing the reaction pathway of propane oxidation revealed that for stoichiometric conditions and at 750 K, the major path for propane oxidation begins with H-abstraction by OH and HO2 (R1 & R2). If the H-abstraction results in an iC3H7 radical, it will add to molecular oxygen to give iC3H7OO, which later decomposes to propane. If R1 and R2 yield nC3H7, then decomposition to ethene is favoured compared to addition of nC3H7 to molecular oxygen.