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Publication date:
2017

Document Version
Peer reviewed version

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Citation (APA):

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Propane Oxidation at High Pressure and Intermediate Temperatures

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Abstract

Propane, a major component in LPG, is reviewed and introduced in the present work. The fuel oxidation started at 700–725 K for a fuel-lean mixture (reducing conditions), and propane concentration dropped sharply at T>725 K for a fuel-lean mixture (oxidizing conditions), and the major detected products have been CO, C3H6, CH4, and C2H4. The model was able to reproduce the onset of fuel oxidation. The H-abstraction by CH3OO from propane (R3) is also sensitive for reducing conditions. The reaction between C3H8 and OH (R2) is also sensitive. While the branch to iC3H7 inhibits the oxidation, the other branch to iC3H7 shows a larger sensitivity compared to the other one (except for oxidizing conditions). The reaction between C3H8 and OH (R2) 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 iC3H7 inhibits the oxidation, the other branch to iC3H7 shows a larger sensitivity compared to the other one.

Introduction

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Results: stoichiometric mixture

Chemical kinetics model

H2/CO/HC’s subsets from recent work by Glarborg et al. [1—4]. The fuel conversion was slightly underpredicted by the model. Sensitivity analyses revealed the importance of H-abstraction reactions by HO2, OH, and CH3OO in controlling propane oxidation at high pressure. 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 high pressure. 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 high pressure. 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 high pressure. 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 high pressure. 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 high pressure. 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 high pressure.

Results: fuel-lean mixture

Motivations

Propane: a major component in LPG
Propane: a minor but sensitive component of natural gas
Temperature of ignition accurately but it seems that CO oxidation to CO2 at high temperatures was not precisely captured by the model.

Experimental: laminar flow reactor
Quartz reactor to minimize surface reactions
Steel pressure shell to achieve high pressures
Isothermal Zone Length: 42—44 cm
Residence time: 8—11 s
Pressure: 100 bar

Summary

Propane Oxidation at Intermediate Temperatures

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References