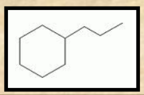
The Low to Intermediate Temperature Oxidation of n-Propylcyclohexane in a Pressurized Flow Reactor

Julius Corrubia, Farinaz Farid, Nicholas Cernansky, David Miller
Department of Mechanical Engineering and Mechanics, Drexel University, Philadelphia, PA 19104

1. MOTIVATION & BACKGROUND

•Department of Defense (DoD) mandated JP-8 jet fuel as the single fuel forward for all military applications, to the extent possible.
-Includes running JP-8 with compression ignition (CI) engines in ground applications, as well as flight.
-United States Air Force is military's largest consumer of JP-8.
•Future advanced propulsion systems will utilize model simulations for design and thus chemical kinetic mechanisms are required for full simulations coupled to computational fluid dynamic (CFD) codes.
•The chemical composition of JP-8 is very complex.
-JP-8 consists of hundreds, if not thousands of hydrocarbon compounds.
-Compounds range in carbon numbers and chemical classes.
•To gain understanding of JP-8 combustion, properly selected surrogate mixtures of fewer components are studied.
-2-10 surrogate components comprise mixture.
-n-propylcyclohexane (n-PCH) is a surrogate component that represents the cycloalkane chemical class for JP-8.
-Coal derived JP-8 from a hydro treating process contains on average 97.3% cycloalkanes.

n-propylcyclohexane, n-PCH (C_9H_{18})



2. OBJECTIVES

•Improve our ability to simulate real fuel combustion in design of future air-breathing propulsion devices.
•To accomplish the objectives three research tasks have been identified:
(1) Understand and quantify combustion properties of real fuels.
(2) Select appropriate surrogate components.
(3) Develop detailed reaction kinetic models and strategies for model reduction.

3. EXPERIMENTAL FACILITIES

- **Pressurized Flow Reactor (PFR)**
- **Gas Chromatograph / Mass Spectrometer / Flame Ionization Detector (GC / MS / FID)**

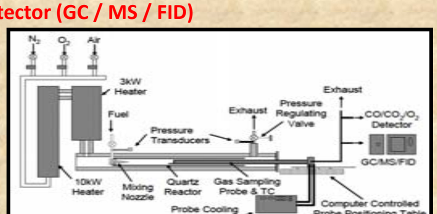


Fig. 1 - PFR Schematic

4. EXPERIMENTAL METHODOLOGY

•The PFR is designed to study the effects of temperature and pressure on the oxidation of hydrocarbon fuels with relative isolation from fluid mechanics and temperature gradients.
•PFR experiments are conducted using the Direct Transfer Controlled Cool Down (DT-CCD) methodology.
-PFR is pre-heated to the maximum reaction temperature of approximately 850 K.
-Once PFR maximum reaction temperature is stabilized the first sample is extracted and the controlled cool down begins.
•PFR samples extracted at selected temperatures with the sample probe and then injected into GC / MS / FID for online analysis.
-Identification and quantification of unknown species from GC / MS / FID performed with retention time matching, mass spectrum matching (NIST '08) and chromatogram analysis.

Fig. 2 - PFR Photo

Fig. 3 - GC / MS / FID Photo

5. RESULTS AND DISCUSSION

Parameter	Value
n-PCH molar fraction	758 ppm
O_2 molar fraction	42100 ppm
N_2 molar fraction	Balance
Equivalence Ratio (φ)	0.24
Temperature	550-850 K
Pressure	8.0 atm
Residence Time	120 ms

Table 1 - Initial experimental conditions for n-PCH

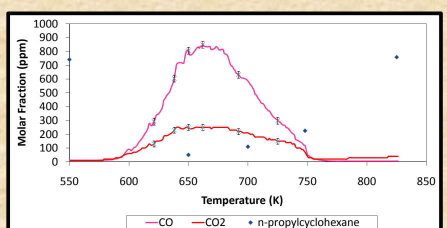


Fig. 4 - Reactivity map for n-PCH

•Discussion (Fig. 4):
-CO is a good indicator of reactivity in the low to intermediate temperature regime. Refer to Fig. 4 for CO production (pink line) during n-PCH oxidation.
-Temperature Increase, Reactivity Decrease due to competing reaction pathways defines Negative Temperature Coefficient (NTC) Behavior.
-n-PCH NTC begins at approximately 660 K with a CO molar fraction of 850 ppm.

6. SELECTED RESULTS

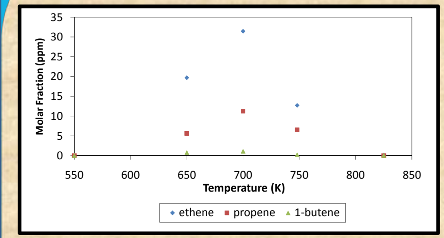


Fig. 5 - Key alkenes produced from n-PCH

•Discussion (Fig. 5)
-Alkenes peaked ne
NTC start.
-Ethene and prope
likely formed from
propyl alkyl side ch
of n-PCH.

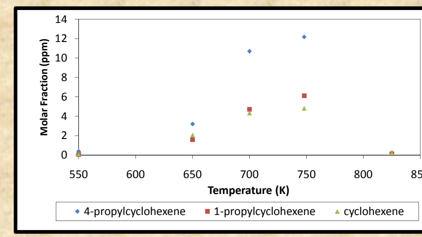
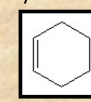


Fig. 6 - Key cycloalkenes produced from n-PCH

•Discussion (Fig. 6)
-Cycloalkenes peal
at about 750 K in t
intermediate
temperature regim

cyclohexene



7. SELECTED RESULTS

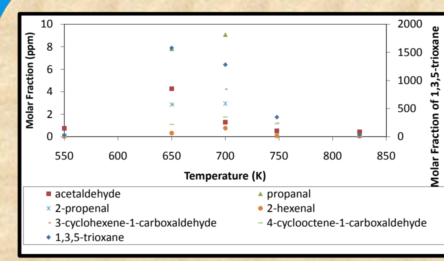


Fig. 7 - Key aldehydes produced from n-PCH

•Discussion (Fig
-Aldehydes pea
near NTC start.
-1,3,5-trioxane
accounted for a
25 % of initial
carbon.

8. SUMMARY AND FUTURE WORK

•Low to Intermediate temperature (550-850 K) oxidation of n-PCH was studied in a
at lean conditions, pressure of 8 atm and constant residence time of 120 ms.
•Reactivity, as indicated by CO production, exhibits classical NTC behavior.
•Intermediate species identified and quantified with GC / MS / FID.
•Intermediate species observed by class include: straight chain alkenes, cycloalkene
aldehydes, ketone-substituted cycloalkanes, carboxylic acid, two-ring structures.
•Carbon balances ranged from 70%-100%. Seventy intermediate species measured
•Oxidation behavior of n-PCH is very similar to results obtained from n-BCH oxidatic
•Future experiments with n-PCH will be done at higher fuel loading to increase the
magnitude of intermediate species production. Further experiments to be perform
establish reproducibility and error estimation for kinetic modeling.

Research supported by the Air Force Office of Scientific Research under Grant No. FA9550-08-1-0040 (AFRL Ener