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Oxidation of 2,7-Dimethyloctane and *n*-Propylcyclohexane in the Low to Intermediate Temperature Regime with a Pressurized Flow Reactor

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The Pressurized Flow Reactor (PFR) at Drexel University was used to study the low to intermediate temperature oxidation of 2,7-Dimethyloctane (2,7-DMO) / air and *n*-Propylcyclohexane (*n*-PCH) / air. 2,7-DMO is a symmetric lightly branched alkane (an isomer of *n*-Decane) and *n*-PCH is a cycloalkane; both are possible surrogate components of their respective chemical classes commonly used for chemical kinetic model development and validation. The experimental conditions studied were: temperature of 550-850 K; pressure of 8.0 atm; residence time of 120 ms. The initial hydrocarbon mole fractions were: 843 ppm 2,7-DMO (equivalence ratio of 0.31) and 824 ppm *n*-PCH (equivalence ratio of 0.27). The oxidation intermediates were extracted from the PFR and then identified and quantified with a Gas Chromatograph / Flame Ionization Detector (GC / FID) coupled to a Mass Spectrometer (MS). Carbon monoxide (CO) levels were measured online to monitor fuel reactivity and map the Negative Temperature Coefficient (NTC) regime. For *n*-PCH oxidation NTC start was at approximately 690 K, as indicated by maximum CO and minimum O₂ mole fractions. Over 60 intermediate species were measured and carbon balances were greater than 90% for all sample temperatures. Similar intermediates were previously measured for *n*-Butylcyclohexane (*n*-BCH) oxidation which suggests that similar reaction pathways exist between *n*-PCH and *n*-BCH, as expected. For 2,7-DMO, NTC start was approximately 695 K. Overall fuel reactivity was less than *n*-Decane, likely resulting from the methyl group substitution. Carbon balances were higher than 70% with about 50 intermediate species measured. During the oxidation of 2,7-DMO, high levels of butene were produced near the NTC region. Lower reactivity of 2,7-DMO in comparison to *n*-Decane and *n*-BCH can be explained by the high stability of butene.

1. Introduction

The United States Department of Defense Directive 4140.43 mandated the use of JP-8 jet fuel as the single fuel forward in applicable combustion systems (U.S. Army Tank-Automotive and Armaments Command 2001). The chemical composition of JP-8 varies widely depending on the sources from which the jet fuel is derived. *n*-Alkanes are the primary components of petroleum derived JP-8; whereas JP-8 produced via the Fischer-Tropsch process contains nearly 100% *n*-alkanes; and JP-8 from a coal liquefaction process consists of nearly 100% cycloalkanes. Due to the numerous chemical classes and number of species that exist in real JP-8 jet fuel, the combustion community has come to accept the surrogate fuel approach for exploring the

combustion behavior of real fuels. This approach assumes that a suitable surrogate fuel reproduces the global combustion properties and reaction kinetics similar to the real fuel within a given tolerance. Suggested surrogates range from a single hydrocarbon, such as *n*-heptane, to a dozen pure components. One model for developing surrogate components is to choose hydrocarbons characteristic of the typical structures in real fuels (Dooley 2010; Dooley 2012). Following this suggestion, 2,7-Dimethyloctane (2,7-DMO) and *n*-Propylcyclohexane (*n*-PCH) were selected for investigation in this study.

Only a small number of studies exist for oxidation of 2,7-DMO. The current study is one of the very first investigations of low to intermediate temperature oxidation of 2,7-DMO at elevated pressure (Hanson). Previously, *n*-PCH has been studied in the Drexel University Pressurized Flow Reactor at low to intermediate temperatures and elevated pressures (Corruba). Also, *n*-Butylcyclohexane (*n*-BCH) has been studied in the flow reactor at similar conditions as the *n*-PCH studies (Natelson 2011). While studies of cyclohexanes have been reported previously (Colket ; Lemaire 2001; Ristori 2001; Mati 2007; Pitz 2007; Silke 2007; Daley 2008; Mittal 2009; Sivaramakrishnan 2009; Vanderover 2009; Vasu 2009; Yang 2009; Crochet 2010; Pousse 2010), the current study is one of only a few studies in the low to intermediate temperature regime and elevated pressure (Crochet 2010). *n*-BCH was oxidized in the Drexel Pressurized Flow Reactor with an initial fuel molar fraction of 1082 ppm ($\phi = 0.38$), temperature of 600-820 K and pressure of 8 atm. Detailed intermediate speciation with a GC / MS revealed straight chain species (i.e. alkenes and aldehydes) and various cyclic compounds (i.e., cycloalkenes, ketone-substituted cycloalkanes and several two ring cyclic structures). This study also revealed the Negative Temperature Coefficient (NTC) behavior that is also characteristic of *n*-alkane oxidation in the low to intermediate temperature regime (Natelson 2011). In another study, a rapid compression machine was used to investigate the auto ignition chemistry of *n*-PCH / air mixtures at lean conditions ($\phi = 0.3, 0.4, 0.5$) with compressed gas temperatures of 620-930 K and pressures ranging from 0.45-1.34 MPa. Stable intermediate oxidation products identified included alkenes, alkynes, cycloalkenes, ketone-substituted cycloalkanes and other more complex structures (Crochet 2010).

2. Experimental Method

The Pressurized Flow Reactor (PFR) at Drexel University was used in this study. Complete details of the methodology, design, construction and installation can be found in (Koert 1990). However, the following provides a summary of the important characteristics of the system. The PFR is a turbulent flow reactor designed to study the low (< 650 K at atmospheric pressure) to intermediate temperature (650-1000 K) oxidation of hydrocarbons with relative isolation from physical phenomena such as gradients in temperature and the flow field. The PFR contains a 22.5 mm ID, 40 cm long quartz reactor tube to provide an environment where surface reactions are negligible. The quartz reactor tube is contained within a stainless steel pressure vessel for pressure elevation up to a maximum of 20 atm. The volume between the quartz reactor tube and pressure vessel forms an annulus that is at the same pressure as the reaction chamber. Synthetic air and high pressure pre-vaporized fuel/nitrogen are introduced into an opposed jet annular mixing nozzle at the inlet to the quartz reactor tube. A water-cooled, borosilicate glass-lined stainless steel sample probe extracts and quenches samples from the centerline of the quartz reactor tube. Figure 1 is a schematic of the PFR equipment and setup.

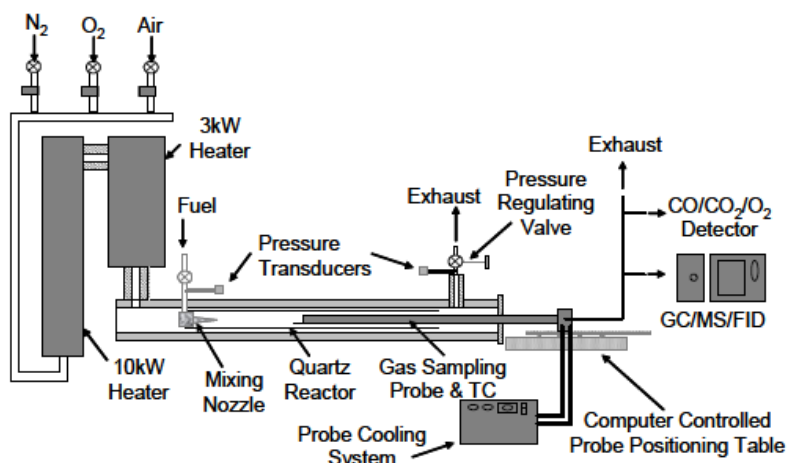


Fig. 1. The PFR schematic.

A Direct Transfer Controlled Cool Down (DT-CCD) operational procedure is used to minimize the time between sample collection and analysis in the GC / MS / FID (Kurman 2011). The PFR is heated to the maximum desired reaction temperature of approximately 850 K using pre-heated air from the circulation heaters. Upon reaching the maximum reaction temperature, fuel is injected into a heated nitrogen stream to ensure vaporization prior to entering the mixing nozzle where it is rapidly mixed with synthetic air in an opposed jet annular mixing nozzle. Further dilution with nitrogen is used to limit temperature rise from heat release. To maintain a constant residence time during the controlled cool down, the sample probe is repositioned for each sample. While the GC/MS/FID analysis is performed on the first sample, the PFR temperature is decreased to the next sample temperature. CO and CO₂ mole fractions are monitored with an on-line, continuous, non-dispersive infrared (NDIR) analyzer and O₂ is measured using an electrochemical oxygen sensor.

The experimental results presented in the following sections are the average of three identical experiments for 2,7-DMO and two identical experiments for *n*-PCH. The experimental conditions for each experiment are shown in Tables 1 and 2. The uncertainty for both hydrocarbon surrogate components studied and stable intermediates measured with the GC/MS/FID is ± 1 standard deviation for the three 2,7-DMO experiments and the two *n*-PCH experiments. The equipment uncertainty for CO and CO₂ is ± 25 ppm, and O₂ is ± 1250 ppm.

Table 1. Test conditions for 2,7-DMO oxidation, residence time 120 \pm 10 ms.

Parameter	Exp 1	Exp 2	Exp 3	Avg	Uncertainty
2,7-DMO, ppm	843	856	830	843	± 13
O ₂ , ppm	42,100	42,100	42,100	42,100	± 1250
N ₂	Balance	Balance	Balance	Balance	-
Equivalence Ratio (ϕ)	0.30	0.32	0.31	0.31	± 0.05
Temperature, K	550-850	550-850	550-850	550-850	-
Pressure, atm	8.000	8.000	8.000	8.000	± 0.025

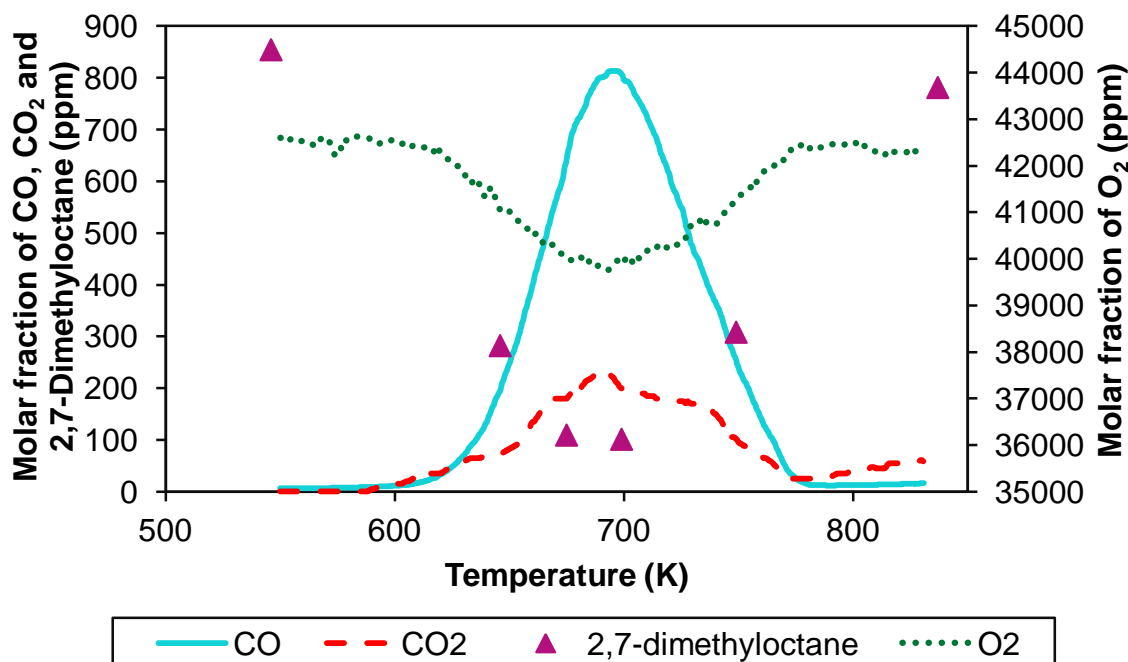
Table 2. Test conditions for *n*-PCH oxidation, residence time 120±10 ms.

Parameter	Exp 1	Exp 2	Avg	Uncertainty
<i>n</i> -PCH, ppm	830	821	826	±20
O ₂ , ppm	42,100	42,100	42,100	±1250
N ₂	Balance	Balance	Balance	-
Equivalence Ratio (ϕ)	0.27	0.27	0.27	±0.05
Temperature, K	550-850	550-850	550-850	-
Pressure, atm	8.000	8.000	8.000	±0.025

3. Experimental Results and Discussion

3.1. 2,7-Dimethyloctane Oxidation

2,7-DMO exhibited classical NTC behavior as indicated by the reactivity map, shown in Fig. 2. NTC behavior is characterized by the decrease of reactivity as temperature increases. The magnitude of reactivity in the experiments was indicated from CO production, since CO does not oxidize significantly to CO₂ in the low to intermediate temperature region (Wilk 1989). The start of the NTC region occurs at about 695 K with a maximum CO molar fraction of 800 ppm. At the start of NTC, maximum fuel consumption occurs with over 90% of 2,7-DMO being converted to intermediate species.

**Fig. 2. Reactivity map for 2,7-DMO oxidation.**

About 50 intermediate species were identified with the GC/MS/FID system and the carbon balance ranged from 70%-100% over the temperature range studied. Figure 3 shows the major alkenes identified and quantified, listed in order of decreasing molar fraction at 750 K were as follows: butene, propene, 2-methyl-1-pentene and ethene. Butene is a major intermediate species produced during the oxidation of 2,7-DMO. The stability of butene is possibly a reason for the lower overall reactivity of 2,7-DMO compared with the straight chain alkane of same carbon number (i.e., *n*-Decane) when comparing CO molar fraction for both fuels at similar experimental conditions in the PFR. The 2-methyl-1-pentene intermediate was possibly produced via C-C bond scission of 2,7-DMO due to the similar chemical structure and methyl group being present in both species.

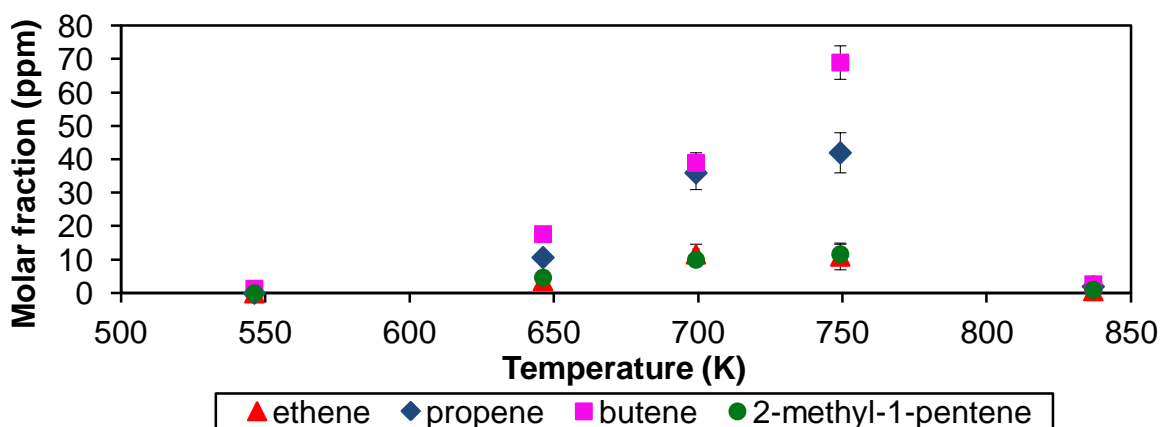


Fig. 3. Key alkenes for 2,7-DMO oxidation.

Key aldehydes measured are presented in Fig. 4. The key saturated aldehydes included iso-butanal, hexanal, and 2-methylpentanal. Among the key unsaturated aldehydes was 2-propenal. Formaldehyde was produced at large quantities representing 36% of carbon fraction at 700 K, where it peaked.

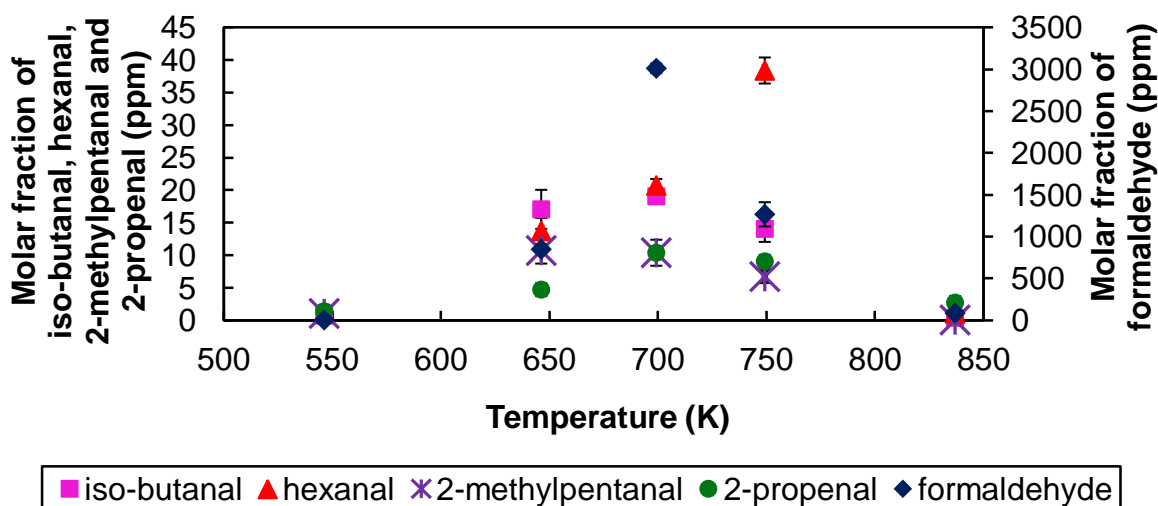


Fig. 4. Key aldehydes for 2,7-DMO oxidation.

Some other select species include acetic acid, octanol, 2-propanone, dihydro-5-methyl-2(3H)-furanone and dihydro-5-pentyl-2(3H)-furanone. Figure 5 is the class analysis of all the intermediate species identified and quantified. In general, it is evident from this chart that alkenes peaked in the NTC region, while aldehydes peaked before NTC start.

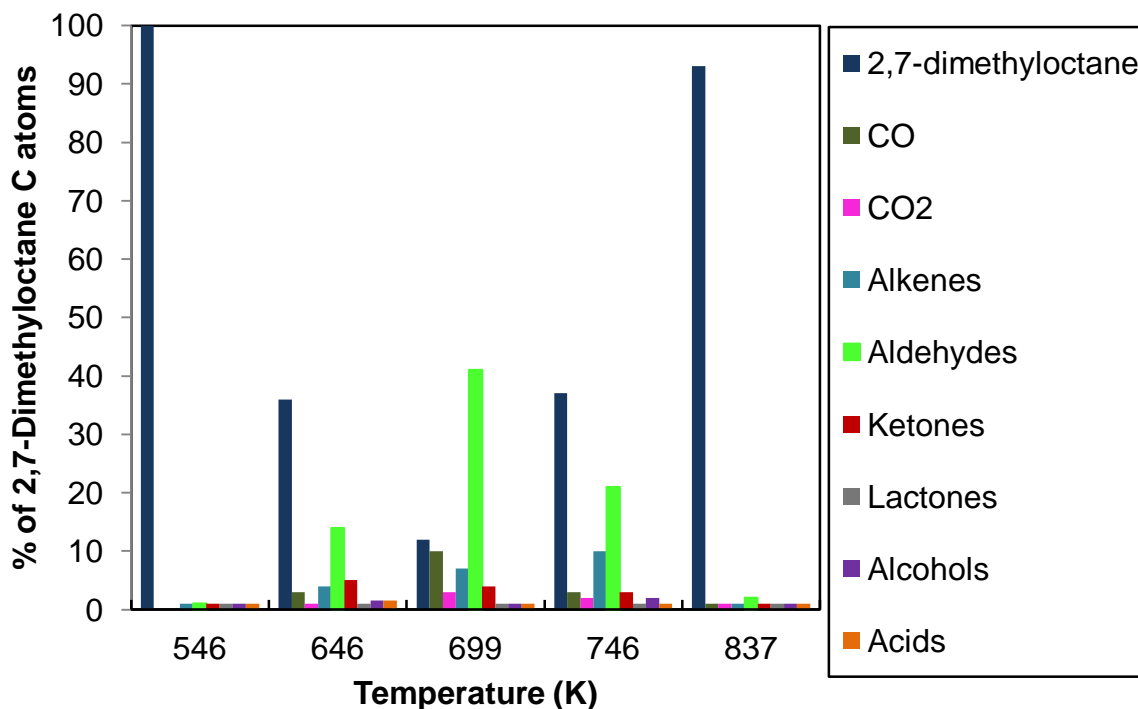


Fig. 5. Chemical class analysis for 2,7-DMO oxidation. Classes accounting for < 1% of total 2,7-DMO carbon atoms are not included.

3.2. *n*-Propylcyclohexane Oxidation

The following results for *n*-PCH oxidation were obtained by performing two PFR experiments at nearly identical conditions, as shown in Table 2. Again, the results shown are the average of both experiments with the uncertainties being ± 1 standard deviation for stable intermediates measured with the GC/MS/FID, and equal to the equipment uncertainty for carbon monoxide, carbon dioxide, and oxygen as shown in Table 2.

Figure 6 represents the reactivity map with the molar fractions of carbon monoxide, carbon dioxide, molecular oxygen, and *n*-PCH plotted with respect to temperature. As with 2,7-DMO, the oxidation behavior of *n*-PCH also possesses classical NTC behavior. The start of NTC for *n*-PCH, as indicated by the temperature at which the molar fraction of CO peaks and begins to decrease, occurs at approximately 700 K with CO production of roughly 770 ppm. Also, carbon dioxide production at NTC start is about 180 ppm which is similar to what has been observed previously with PFR experiments performed on straight chain alkanes such as *n*-Decane and *n*-Dodecane, as well as the currently studied methyl-alkylated alkane, 2,7-DMO. Namely, the carbon dioxide profile tracks the carbon monoxide profile over the low to intermediate temperature regime, but at lower levels on the order of 25%-35% of the CO molar fraction. Lastly, at NTC start where maximum reactivity exists

corresponds to a minimum in the *n*-PCH and molecular oxygen molar fraction profile. At NTC start, the *n*-PCH molar fraction is 115 ppm which translates to 86% of the reactant fuel being consumed, and the O₂ molar fraction is about 40,000 ppm which corresponds to 5% of the reactant O₂ being consumed.

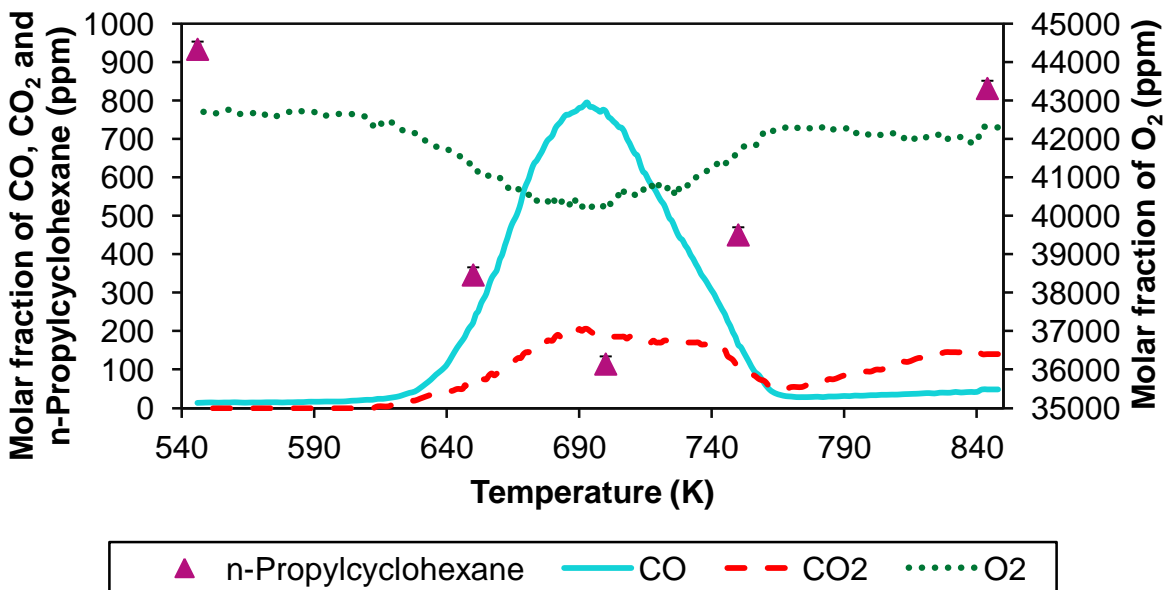


Fig. 6. Reactivity map for *n*-PCH oxidation.

Seventy intermediate species were identified and quantified with the GC/MS/FID system during both experiments. The carbon balances for all sample temperatures were greater than 90%, with the minimum occurring at the 700 K temperature sample point. As with 2,7-DMO, and many other heavy surrogate components studied in the PFR, the lowest carbon balance tends to exist where maximum reactivity occurs. This feature likely can be attributed to the fact that at maximum reactivity there are a larger number of intermediate species that are produced and must be properly accounted for with the GC/MS/FID measurements to maintain acceptable carbon closure. The following plots show the key intermediate species measured at molar fractions greater than approximately 1 ppm.

Figure 7 presents the key linear alkenes measured during *n*-PCH oxidation. In addition to ethene, propene, and butene, pentene, hexene and alkynes (i.e. 2-butyne) were also measured at much smaller molar fractions of less than approximately 1 ppm. The maximum molar fraction of ethene, propene and butene was 31 ppm, 11 ppm and 1 ppm, respectively, and occurred at the NTC start temperature of 700 K. The behavior of the linear alkenes, along with the other intermediate species measured agree very well with previous PFR experiments performed with *n*-PCH at very similar conditions (Corrubia). The data presented for the previous experiments was for only a single experiment, whereas the goal of the current work was to perform nearly identical experiments that can be used to determine the uncertainties for each of the seventy intermediates measured. Also, similar behavior for linear alkenes was observed in prior work done with the Drexel PFR during *n*-Butylcyclohexane (*n*-BCH) oxidation (Natelson 2011). The *n*-BCH experiments revealed that ethene and propene were also produced in the largest quantities near NTC start at 715 K (Natelson 2011). Moreover, 1-butene was also measured to be approximately 10 ppm at 715 K during *n*-BCH oxidation.

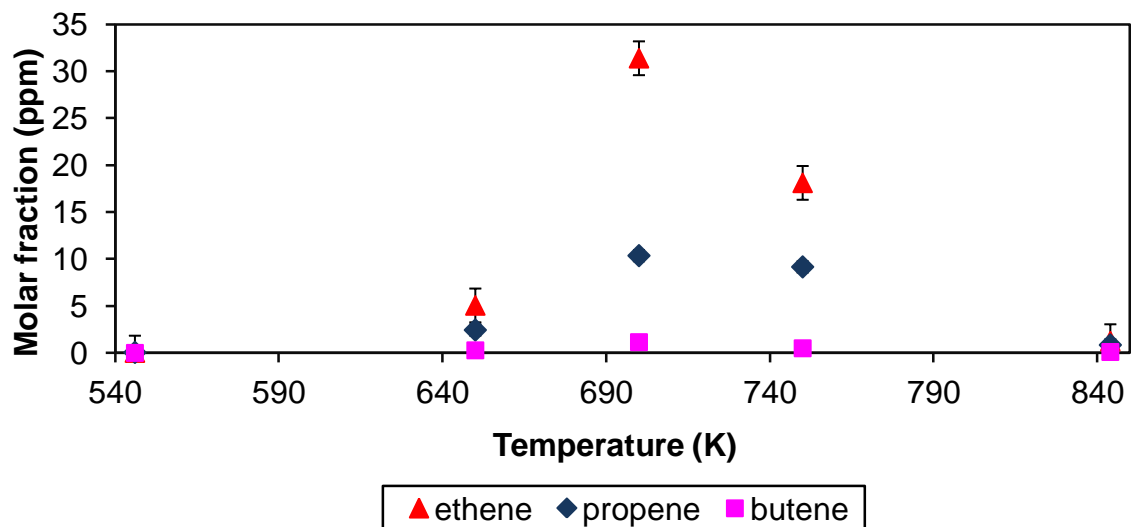


Fig. 7. Key alkenes for *n*-PCH oxidation.

There were also a number of saturated and unsaturated cycloalkane and cycloalkene stable intermediate species measured. Cycloalkenes measured included (listed in decreasing molar fraction at peak): cyclohexene, and cyclopentene which peaked in the NTC regime. Alkane substituted cycloalkanes measured included (listed in decreasing molar fraction at peak): 1-methyl-2-propyl-cyclohexane, and ethylcyclohexane which peaked at NTC start. Alkene substituted cycloalkanes measured included (listed in decreasing molar fraction at peak): methylene-cyclohexane, and methylene-cyclopentane which peaked in the NTC regime. Alkane substituted cycloalkenes measured included (listed in decreasing molar fraction at peak): 4-propyl-cyclohexene, 3-ethyl-cyclohexene, 4-(1,1-dimethylethyl)-cyclohexene, and 4-methylcyclohexene which peaked in the NTC regime.

Refer to Fig. 8 below for the key alkane substituted cycloalkenes measured, which constituted the chemical class with the largest percentage of *n*-PCH carbon atoms reacted at maximum reactivity among the saturated and unsaturated cycloalkane and cycloalkene classes quantified that were mentioned in the previous paragraph. Furthermore, in the NTC regime, particularly at 750 K, the total summation of the saturated and unsaturated cycloalkane and cycloalkene stable intermediate species measured was approximately 10% of the total *n*-PCH carbon atoms reacted (refer to Fig. 10). It is also important to note that at maximum reactivity for the normal cycloalkenes (i.e., cyclohexene and cyclopentene at 750 K) they were produced at approximately 0.5% of the *n*-PCH carbon atoms reacted. Due to the relatively low yield of the cyclic species (i.e., 10% was the maximum which neglects *n*-PCH itself and the small yield of normal cycloalkenes), this possibly suggests that the *n*-PCH molecule's backbone ring opens easily and then decomposes via beta scission into smaller hydrocarbon fragments to form the majority of stable intermediate species (e.g., linear alkenes), rather than remain intact as this would imply that a larger percentage of cyclic species are required to be formed from the reactant. Moreover, these initial hydrocarbon fragments can possibly form the other smaller size stable intermediate species measured, such as carbon monoxide once a sufficient amount oxygen radicals become available.

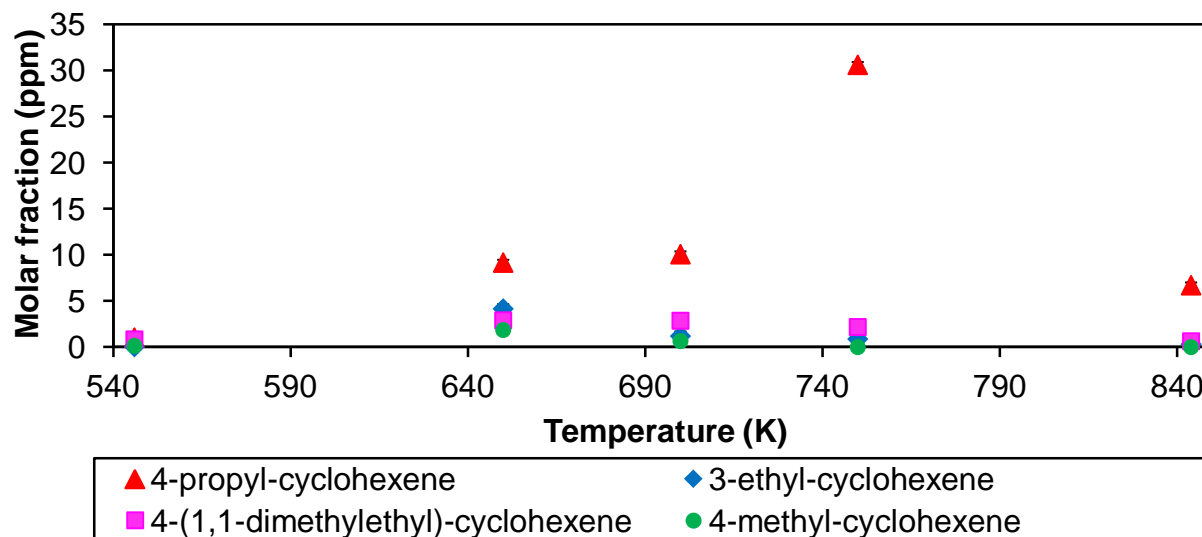


Fig. 8. Key alkane substituted cycloalkenes for *n*-PCH oxidation.

Key aldehydes measured are displayed in Fig. 9. Both saturated and unsaturated aldehydes were identified and quantified. The saturated aldehydes included acetaldehyde, propanal, and butanal while the unsaturated aldehyde shown was 2-propenal. In general, the aldehydes peaked between 650 K and 700 K in the low temperature regime. Also, 1,3,5-trioxane was produced at large molar fractions, likely due to polymerization of formaldehyde. It peaked at 650 K with a molar fraction of approximately 1050 ppm. 3-Cyclohexene-1-carboxaldehyde was measured with a maximum molar fraction of 4 ppm at 700 K. An isomer of this species, namely cyclohex-1-ene-4-carboxaldehyde, was identified in a rapid compression machine experiment performed with *n*-PCH at an equivalence ratio of 0.5, compressed gas temperature of 669 ± 9 K and pressure of 0.7 MPa (Crochet 2010). Other aldehydes measured at lower molar fractions than 3 ppm included 2-hexenal, trans-2-heptenal and 4-cyclooctene-1-carboxaldehyde.

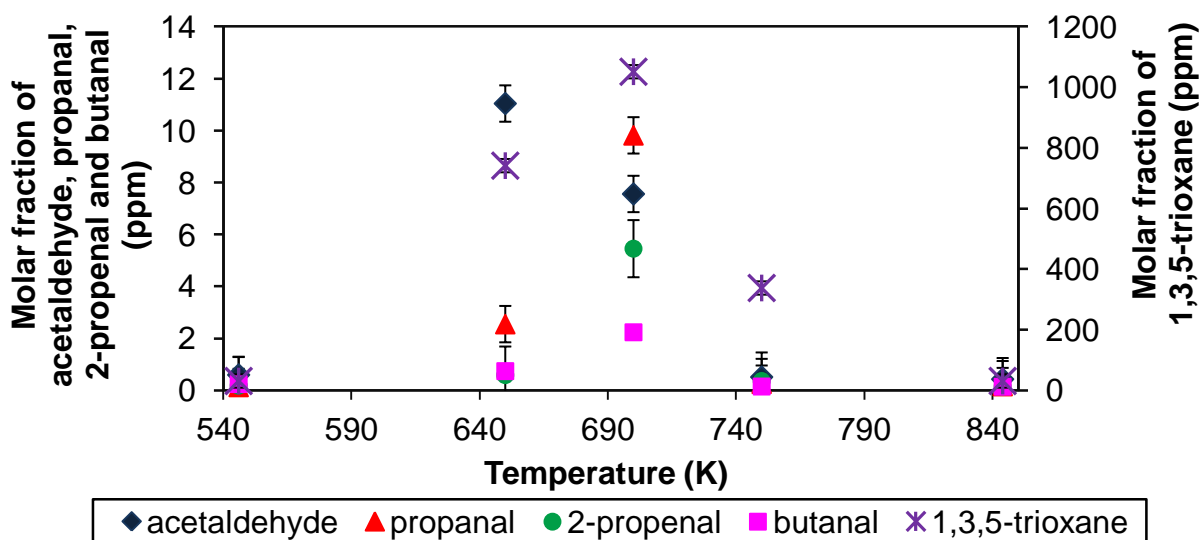


Fig. 9. Key aldehydes for *n*-PCH oxidation.

Other more complex select species included: 4-cyclooctene-1-carboxaldehyde, 2-methylcyclohexyl propionate, cyclohexane, butyldiene and 2-acetonylcyclohexanone. Figure 10 is the class analysis of all the intermediate species identified and quantified. The chart shows that alkenes peaked near NTC start, while aldehydes peaked before NTC start.

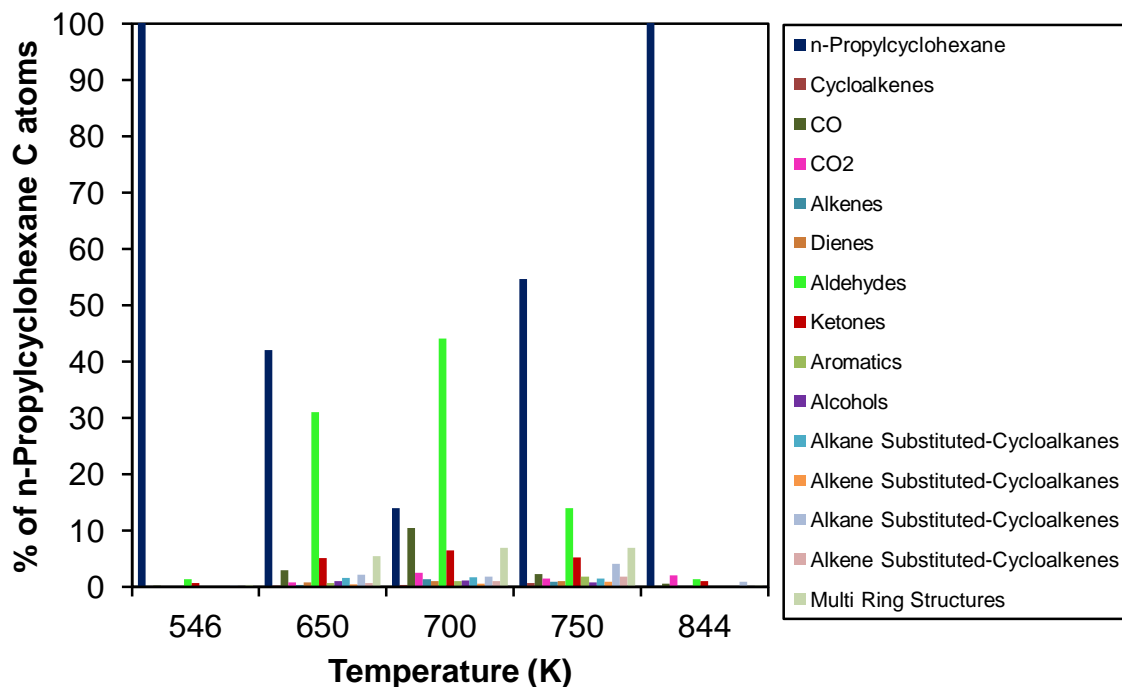


Fig. 10. Class analysis for *n*-PCH oxidation. Classes accounting for < 1% of total *n*-PCH carbon atoms are not included.

4. Conclusions

The low to intermediate temperature (550 K – 850 K) oxidation of 2,7-Dimethyloctane (2,7-DMO) and *n*-Propylcyclohexane (*n*-PCH) was studied in the Drexel Pressurized Flow Reactor at a pressure of 8.0 atm, residence time of 120 ms and lean equivalence ratios. The plan was to measure the intermediate species produced from a representative surrogate component of an alkylated alkane (2,7-DMO) and an alkylated cycloalkane (*n*-PCH). Carbon monoxide, carbon dioxide and molecular oxygen were monitored online and continuously to gauge the level of reactivity across the temperature range for both surrogates. All other intermediate species were identified and quantified with a GC/MS/FID system. Results indicated classical NTC behavior for both surrogate components. Butene is a major intermediate specie produced during the oxidation of 2,7-DMO. The stability of 1-butene is possibly a reason for the overall lower reactivity of 2,7-DMO, as compared to in-house experiments with the straight chain alkane of same carbon number (i.e., *n*-Decane) at similar experimental conditions. The relatively low yield of the cyclic species during *n*-PCH oxidation (i.e., 10% was the maximum which neglects *n*-PCH itself and the small yield of normal cycloalkenes) suggests that the *n*-PCH molecule's ring structure opens easily and then decomposes via beta scission into smaller hydrocarbon fragments to form the majority of stable intermediate species (e.g., linear alkenes), rather than

remain intact. The data obtained provide a tool for future validation of development and modification of kinetic models.

Acknowledgments

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