Flow Reactor Studies of Oxidation and Pyrolysis of Jet Fuel Components at Intermediate Temperatures

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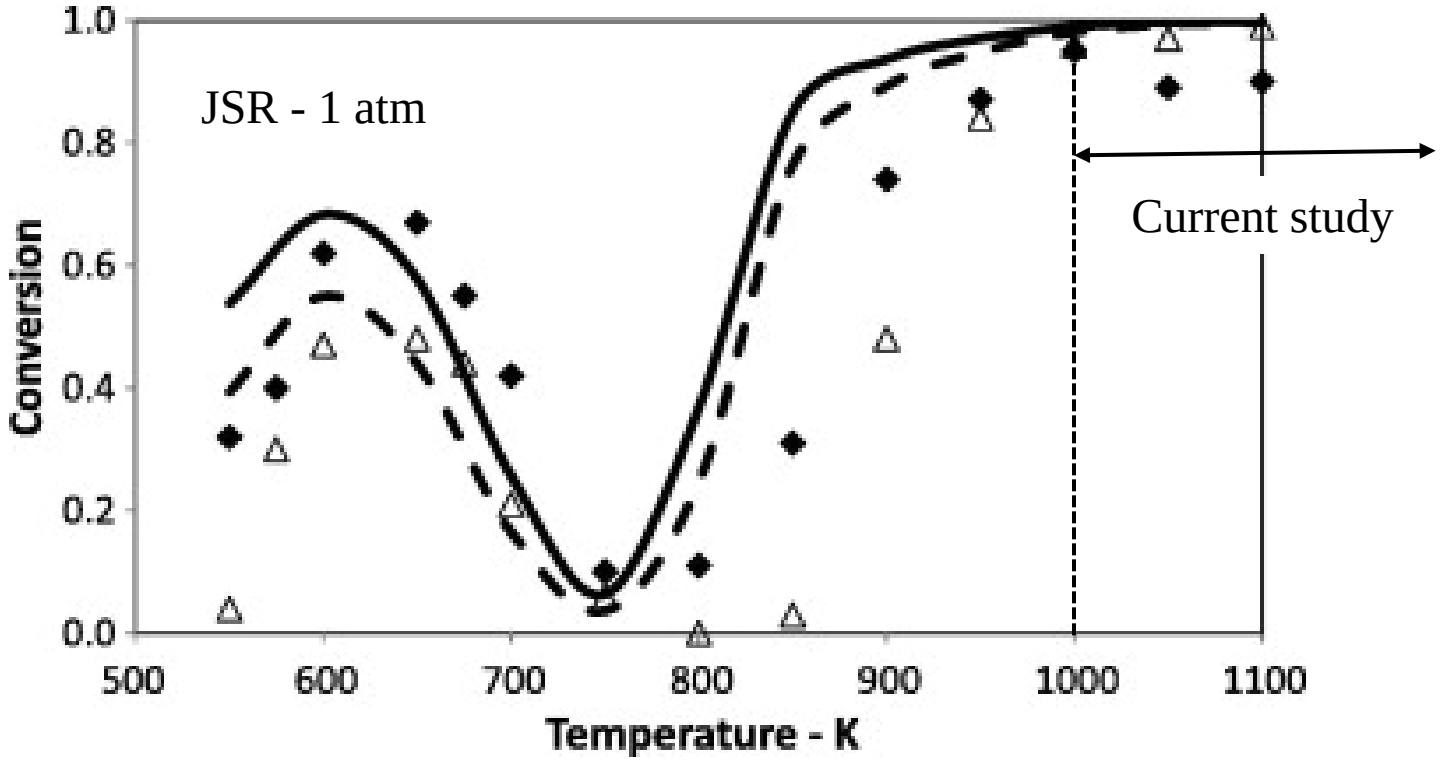
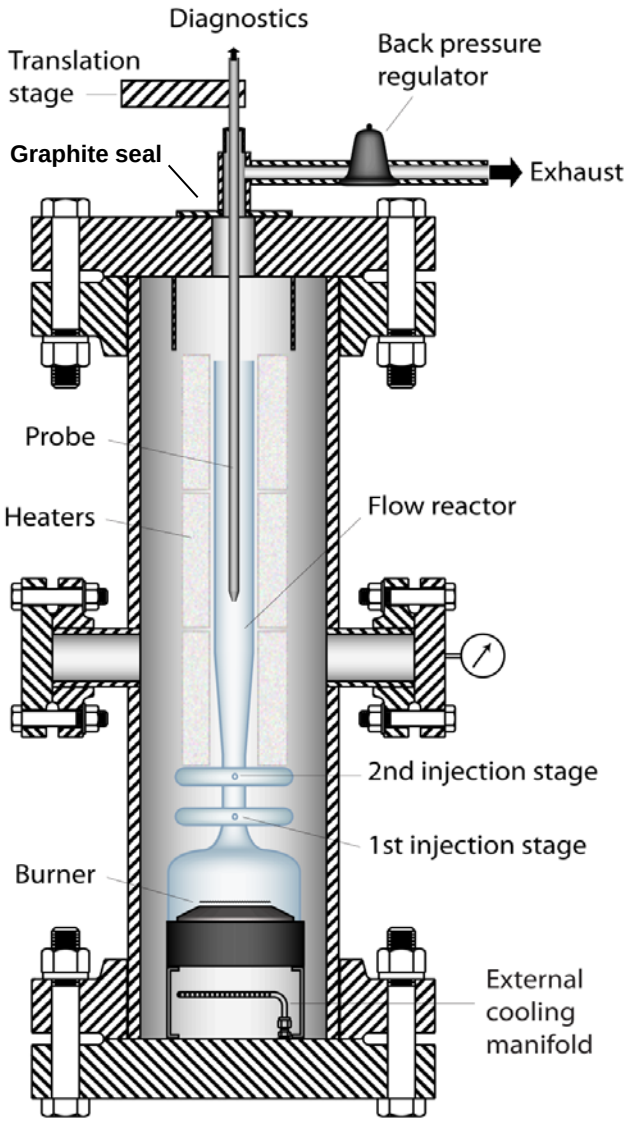
Combustion Regimes of Hydrocarbon Fuels

methyl palmitate ♦, n-decane Δ



Westbrook, et al., *Combust. Flame* 158, 742-755, 2011.

Variable Pressure Flow Reactor



- Pressures 1-10 bar
- T < 1300 K
- Residence times 5-100 ms

Reactor Flow Field Characterization

- Axial and radial mean velocity profiles and turbulence intensity using hot wire anemometry.
- Axial and radial mean temperature profiles using thermocouples.
- Scalar mixing profiles using tracer injection.
- Comparison of data with CFD simulations using Fluent.

Reacting Flow Model

Different approaches to mixing and reaction "time zero" issues:

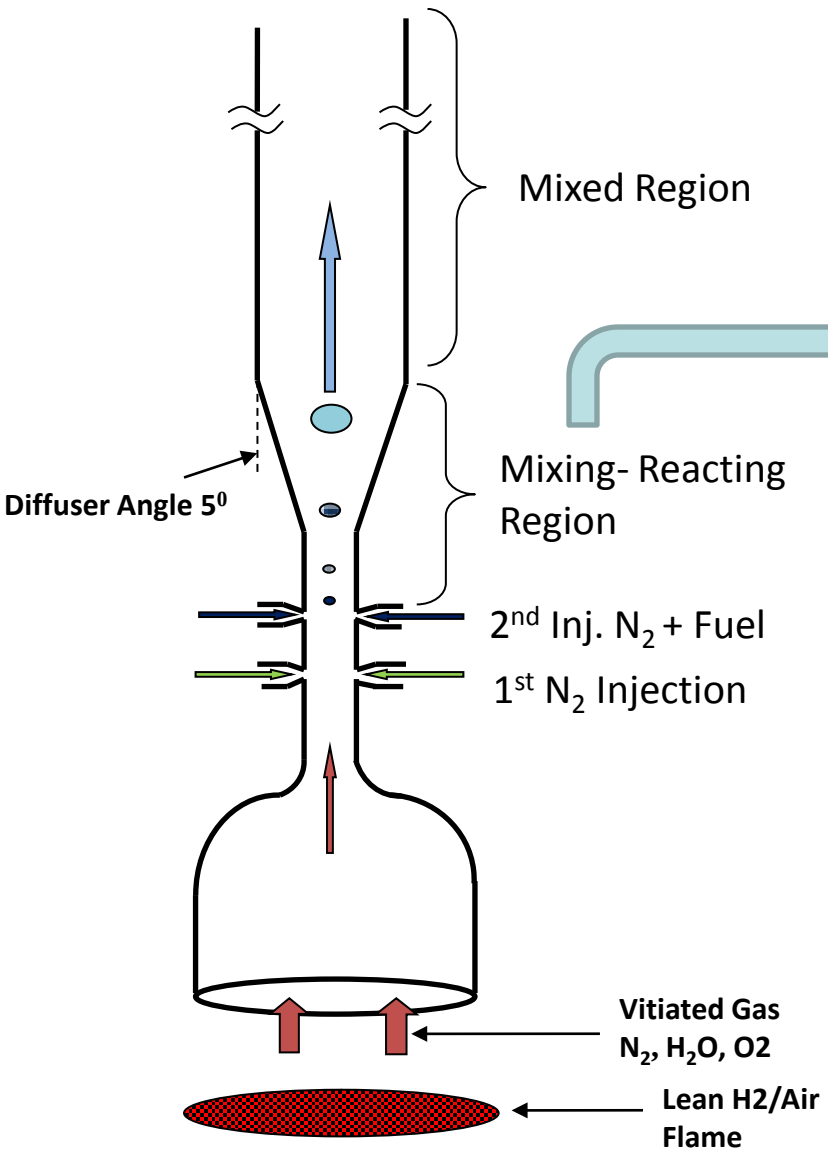
- "Time shifting"
- "Initialization"
- Simultaneous model of mixing and reacting processes

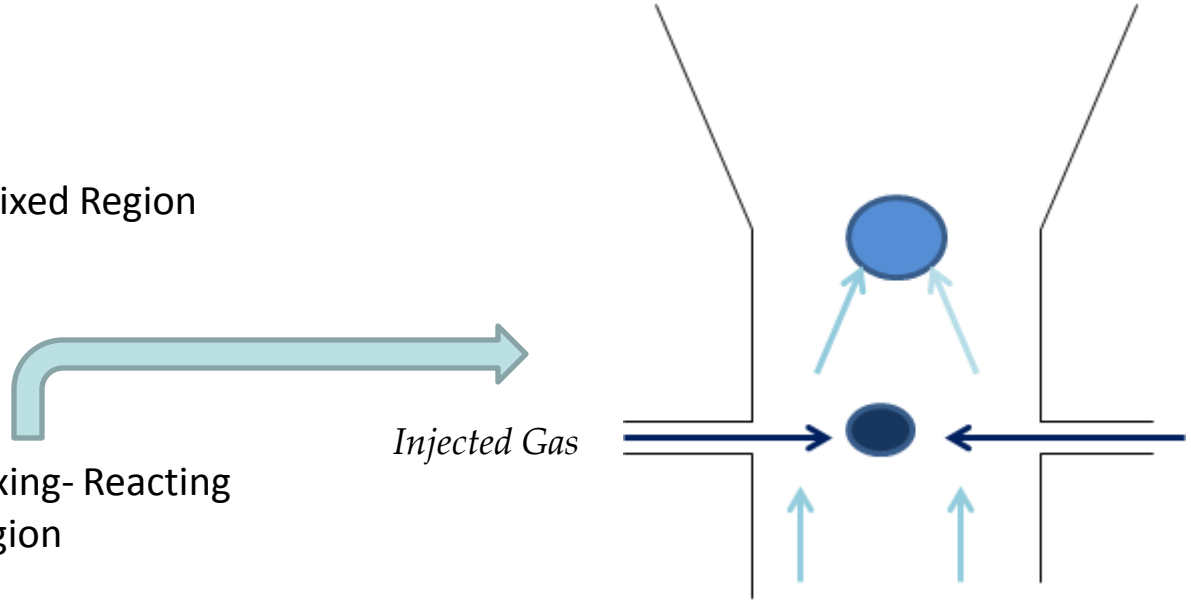
One-dimensional mixing-reacting model based on reactor flow conditions and measured temperature profiles.

Only a single mixing parameter is needed.

Boundary layer correction from centerline velocity measurements.

Reacting Flow Model





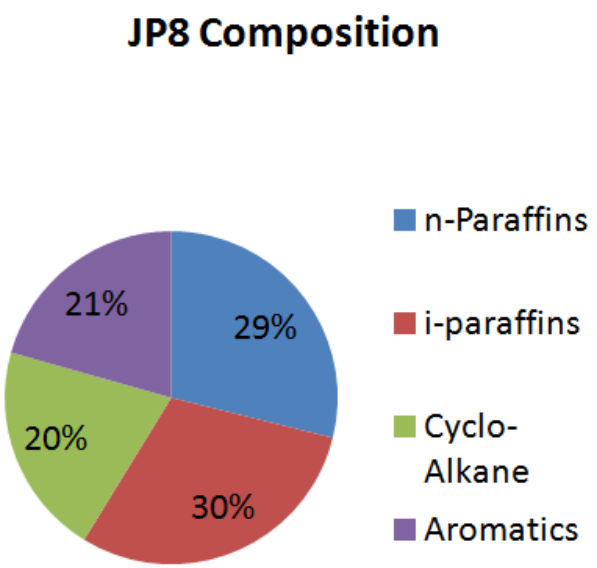
Zwietering Mixing-Reacting Flow Model used to simulate flow – one empirical mixing parameter

Model validated using a single-step irreversible first-order reaction

$$C_2H_5Cl \rightarrow C_2H_4 + HCl$$

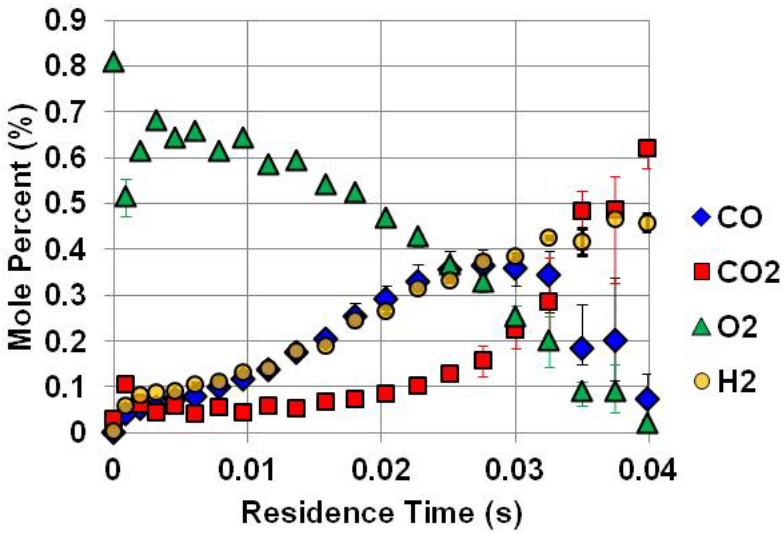
Representative Jet Fuel Properties

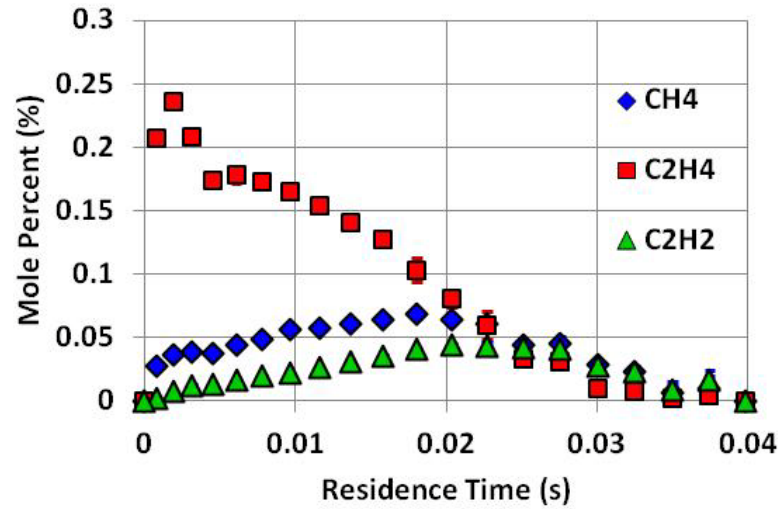
JP8 Property	Value
Molecular Weight	152
Appx Formula	$C_{11}H_{21}$
Boiling Range	140-300 C
Sp. Grav. At 15 C	0.81

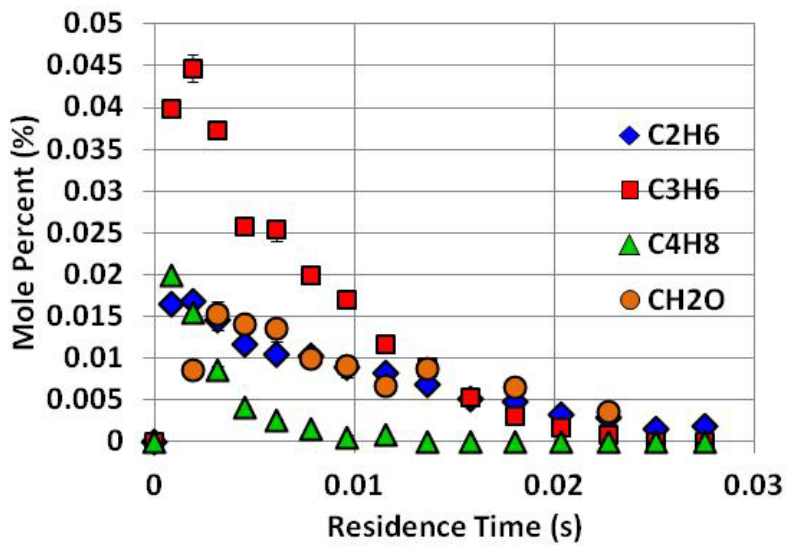


Species Profiles – Oxidation Experiment

$\phi = 1.3$, $T_0 = 1220K$, $P = 1$ bar



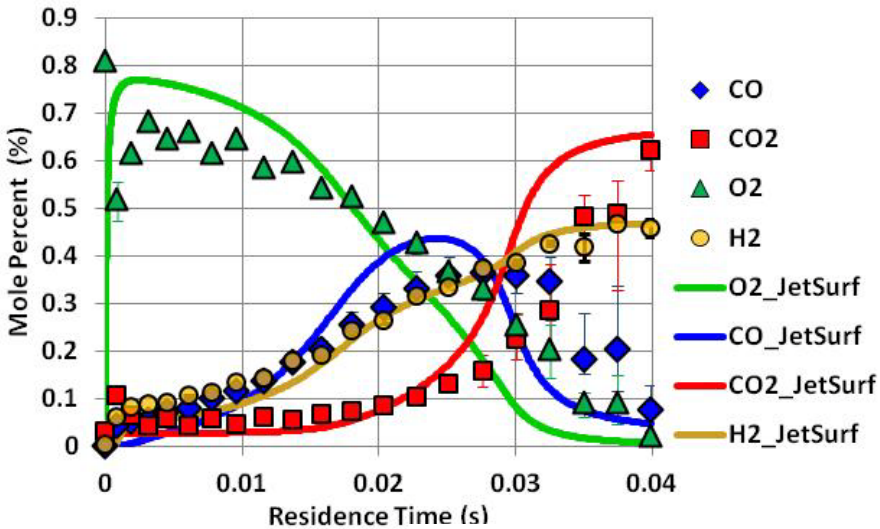


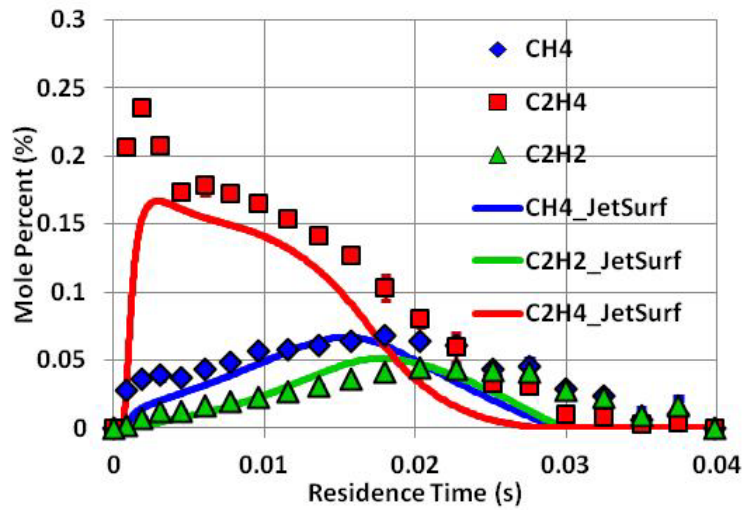


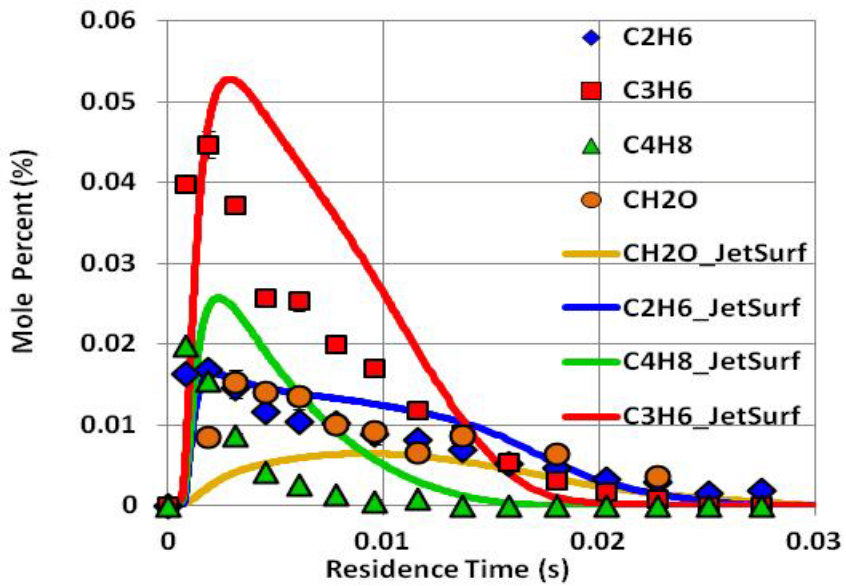
- Rapid reaction of dodecane
- Rapid alkene formation
- Slower formation of CH_4

Species Profiles – Oxidation Experiment

Comparison of data with JetSurf 2.0

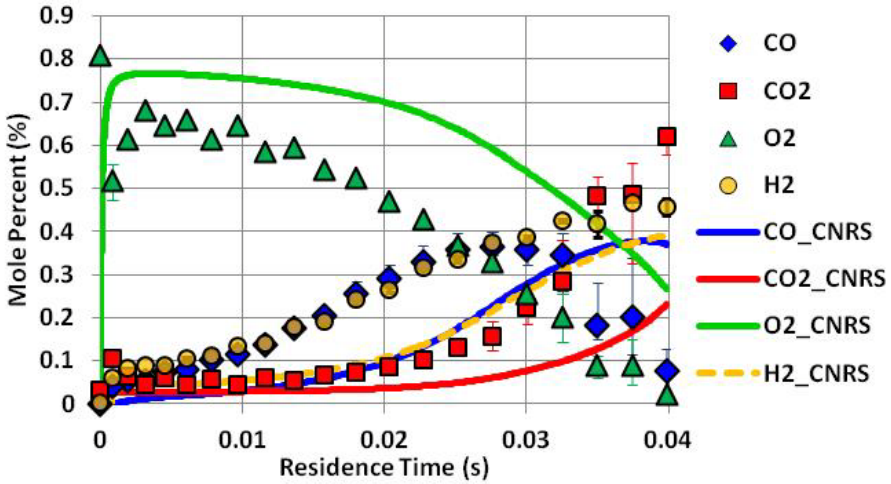


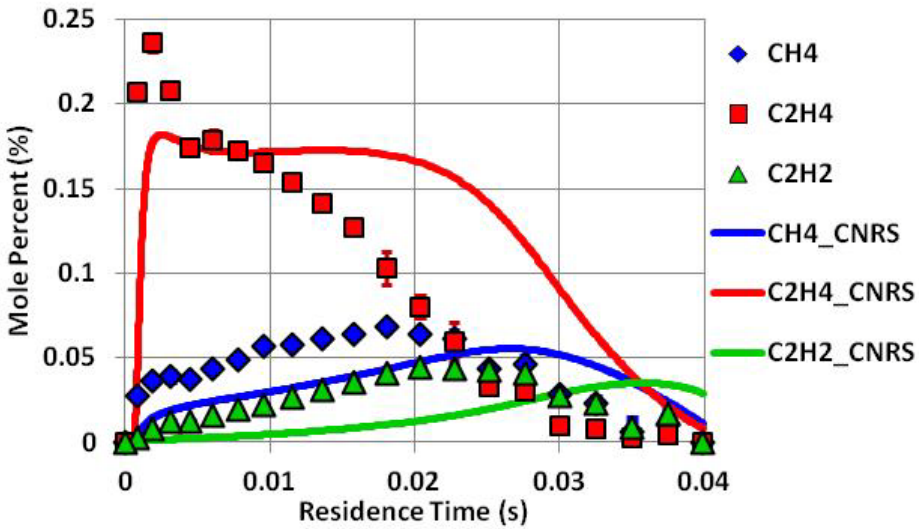


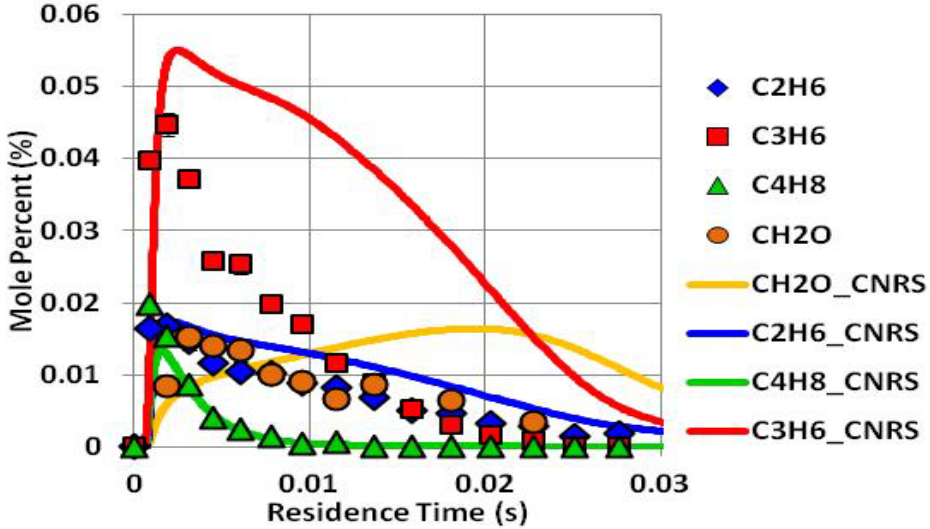


Species Profiles – Oxidation Experiment

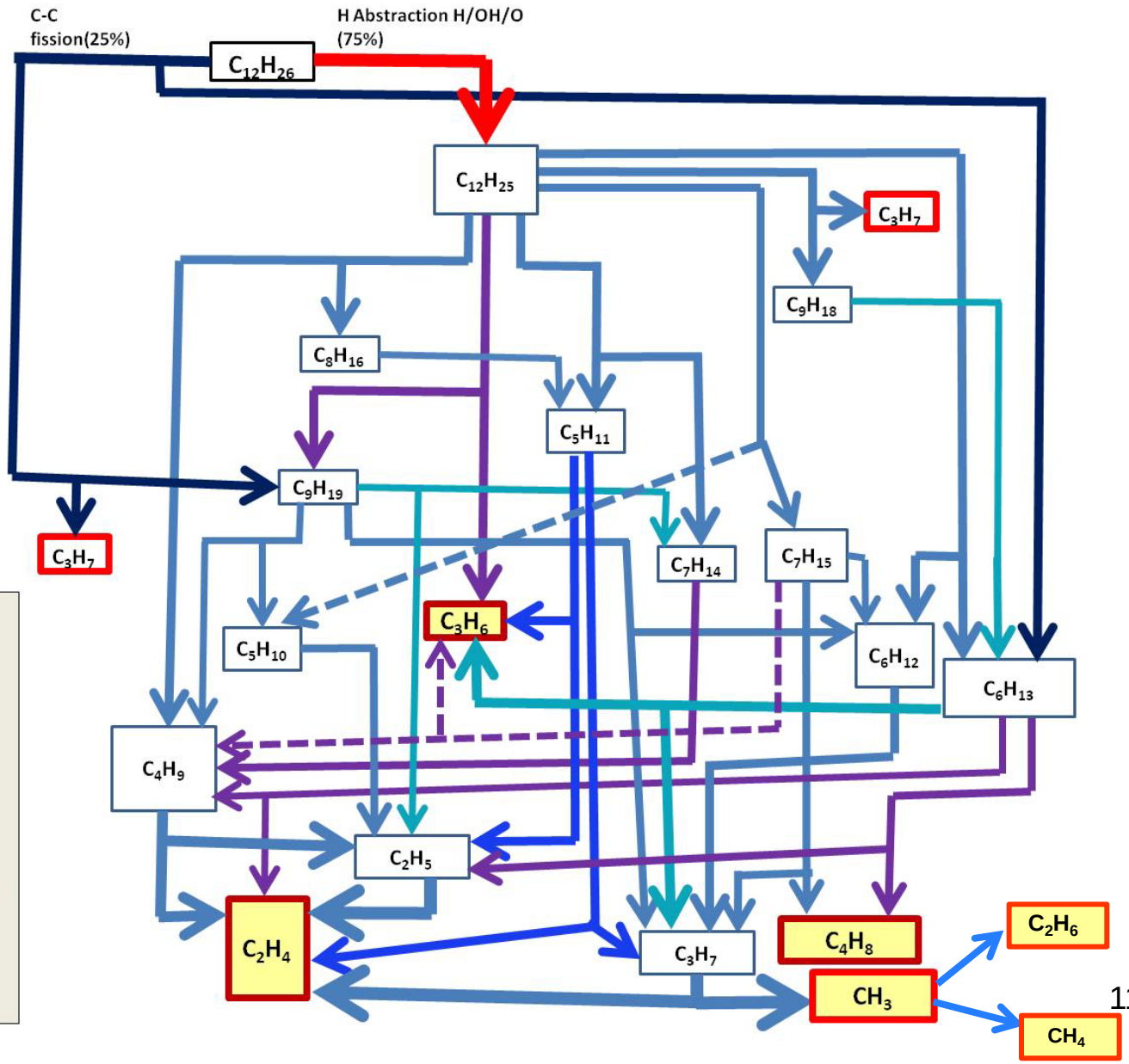
Comparison of data with CNRS Mechanism





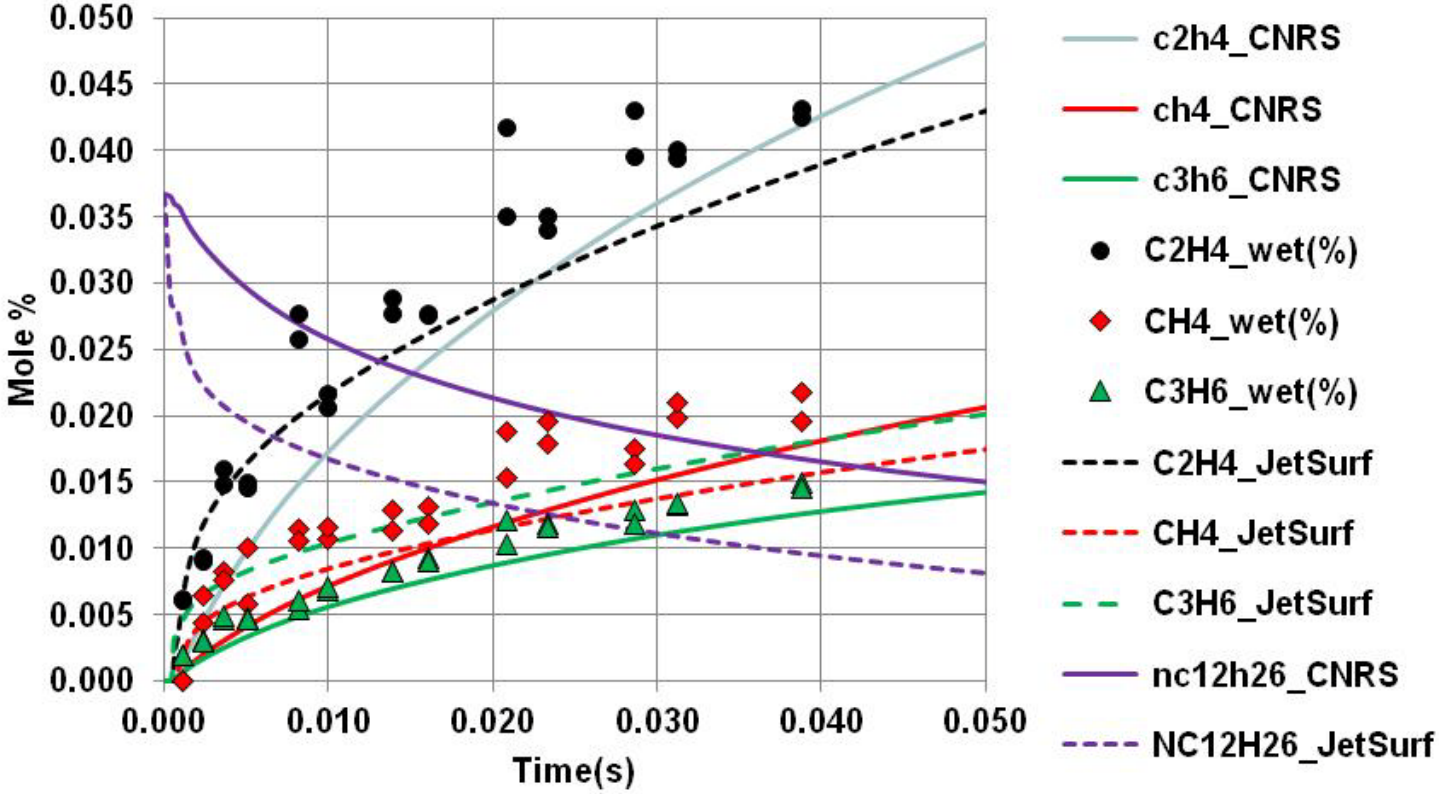


Oxidation Reaction Pathways



1. Dodecane primarily undergoes H-abstraction by O/OH/H to form dodecyl radicals.
2. Dodecyl undergoes β-scission to break into C_4-C_{11} alkenes and corr. alkyl radicals.
3. The higher alkenes undergo pyrolysis or H-abstraction followed by β-scission to break up into smaller alkenes and alkyl radicals.
4. Diagram shows early stages (1ms) when 50% Dodecane has been converted.

Species Profiles – Pyrolysis Experiment



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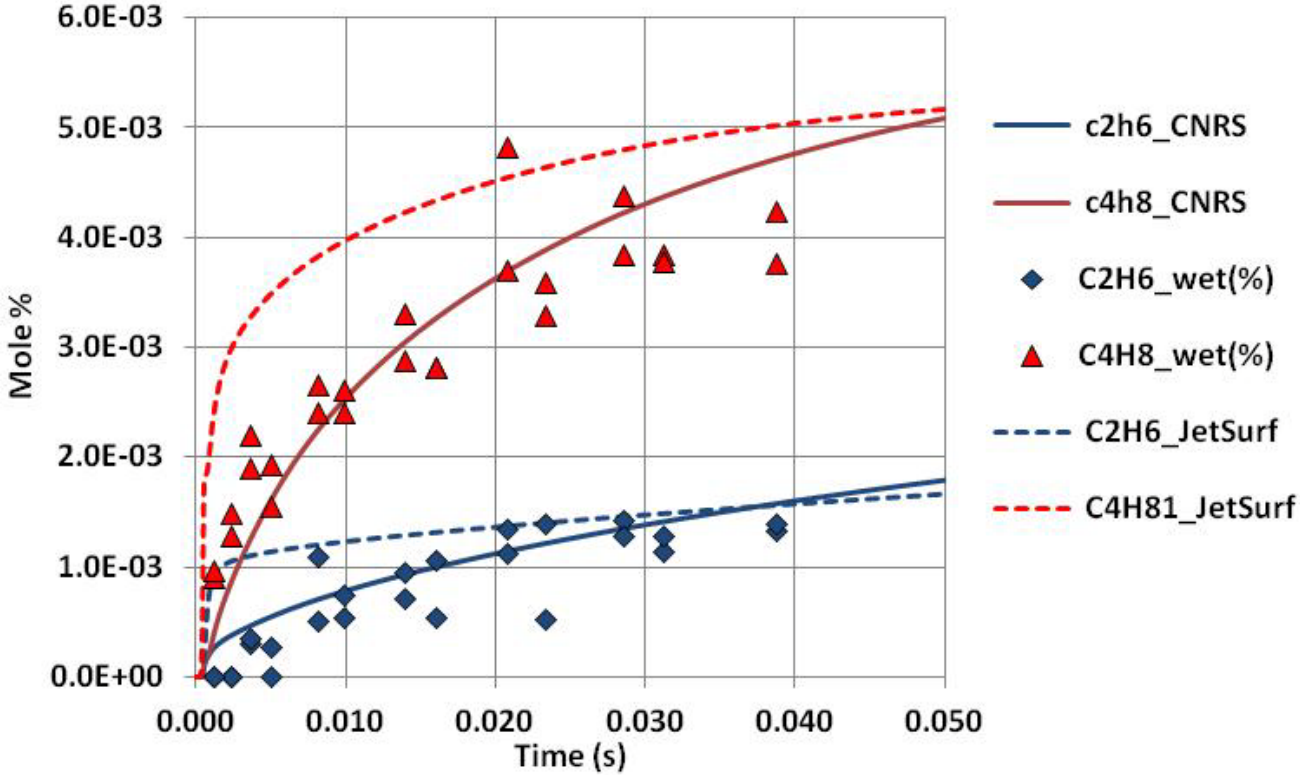
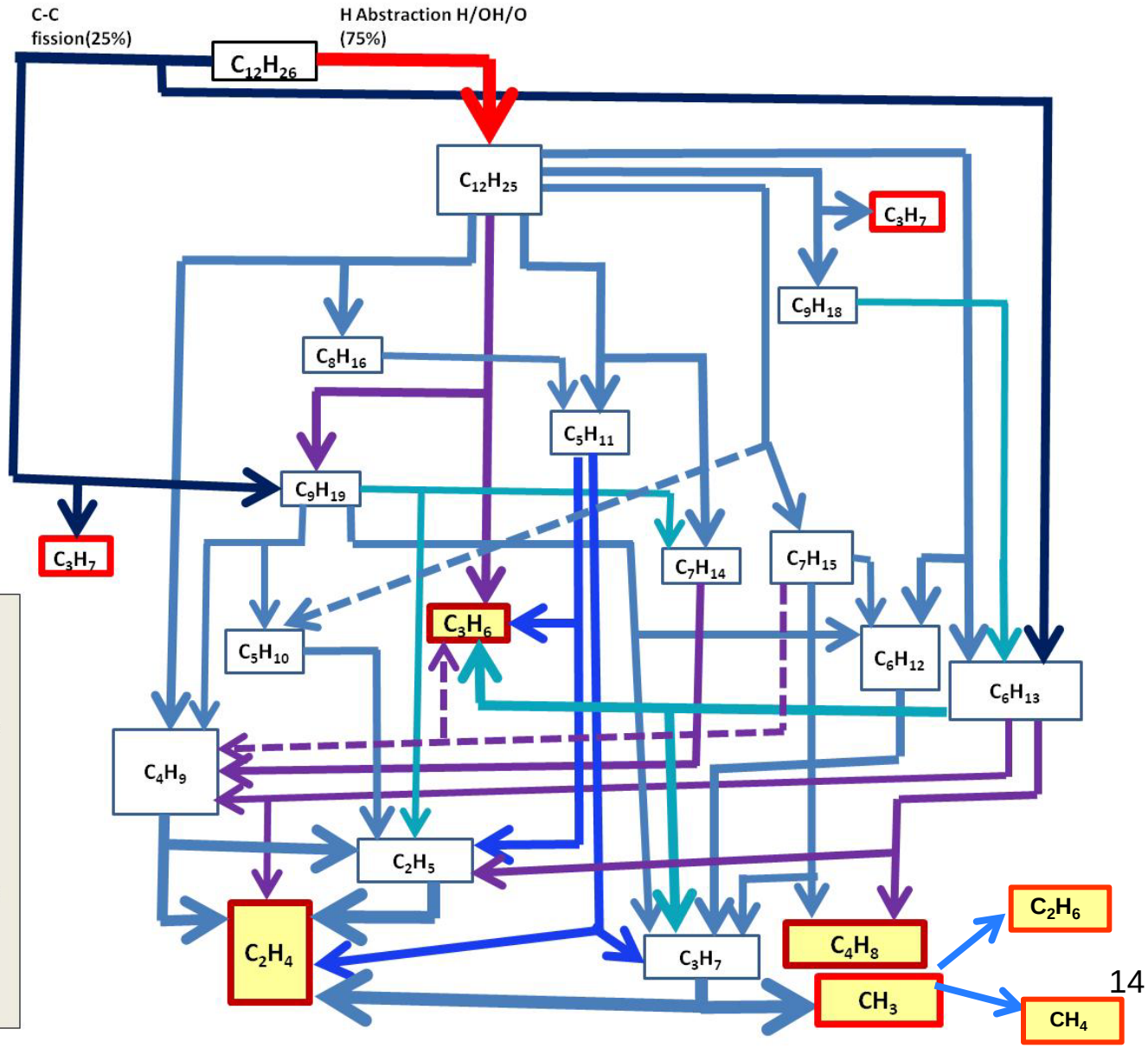


Pyrolysis Reaction Pathways



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Conclusions and Future Directions

- Decomposition of dodecane to alkenes in oxidation experiments at temperatures greater than 1000K is very fast so that heat release (and final product formation) is controlled by oxidation of hydrocarbon fragments from dodecane decomposition.

- The reaction pathways to hydrocarbon fragments are similar in both dodecane oxidation and pyrolysis.

- Future experiments will involve oxidation and pyrolysis of other jet fuel components (cycloalkanes, iso-alkanes and aromatics) to identify reaction pathways and to validate detailed reaction models.