Fuel and Combustion Laboratory (F&C)
Department of Aeronautics and Astronautics

MPOC's Green Technology Innovations webinar

Renewable Jet Fuels

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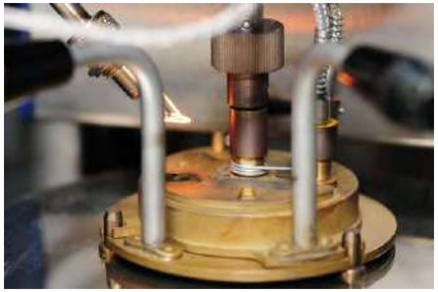
Developing a new fuel

Laboratory development



Fuel Combustion Test

Process Evaluation

Feedstock Solution

Transportation Test

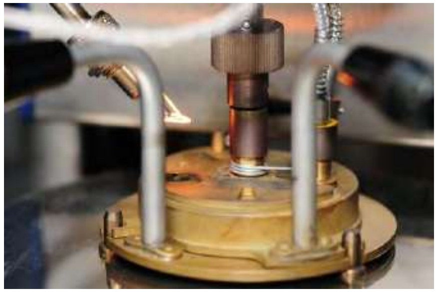
Commercialization

Distribution pipeline

Daily Use

Laboratory Development

Laboratory development



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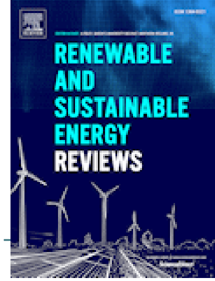
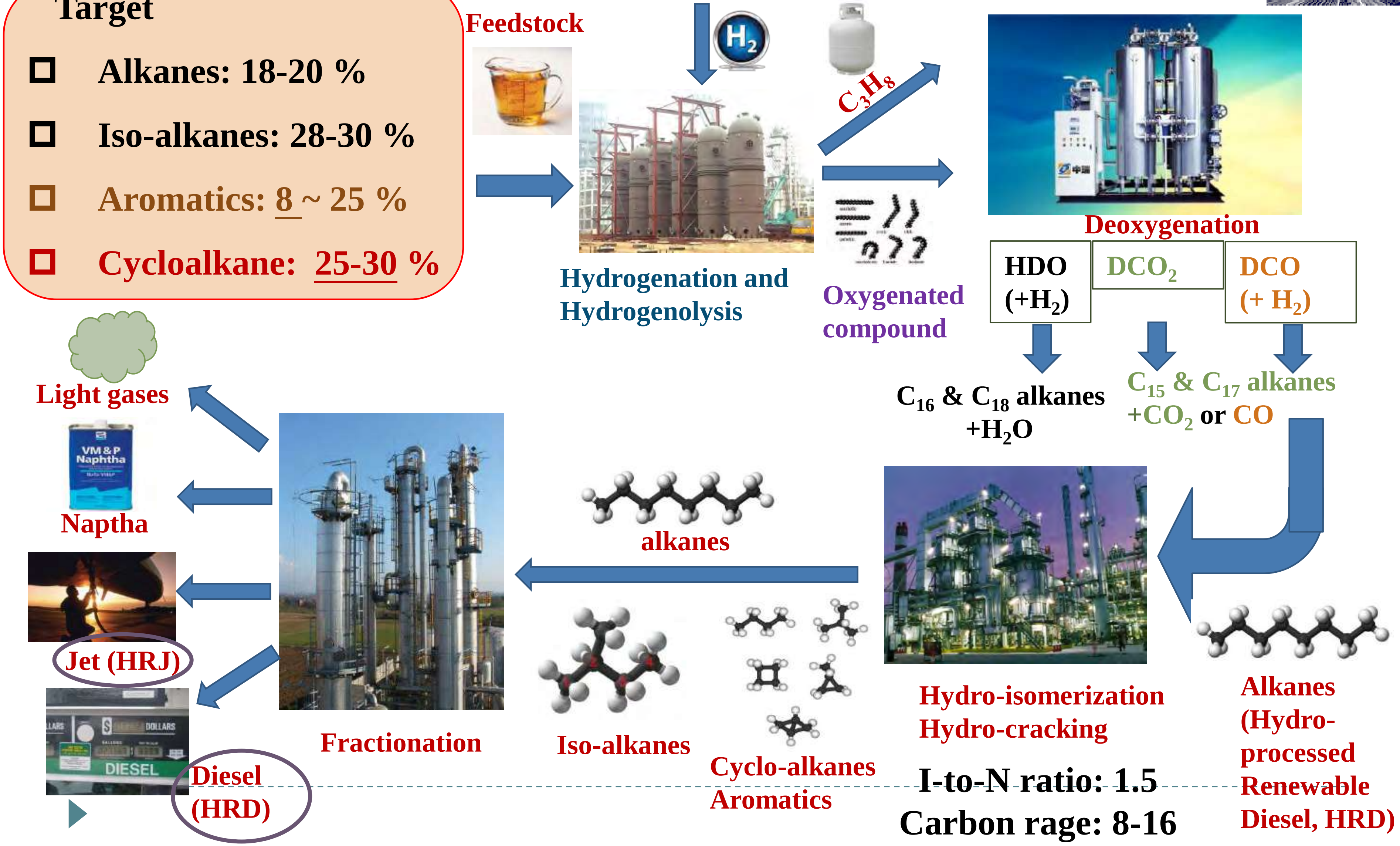


Producing Renewable Jet Fuel

Target

- ☐ Alkanes: 18-20 %
- ☐ Iso-alkanes: 28-30 %
- ☐ Aromatics: 8 ~ 25 %
- ☐ Cycloalkane: 25-30 %



Feedstock

H_2

Hydrogenation and Hydrogenolysis

C_3H_8

Oxygenated compound

Deoxygenation

HDO ($+H_2$)

DCO_2

DCO ($+ H_2$)

C_{16} & C_{18} alkanes $+H_2O$

C_{15} & C_{17} alkanes $+CO_2$ or CO

Alkanes (Hydro-processed Renewable Diesel, HRD)

Hydro-isomerization
Hydro-cracking

I-to-N ratio: 1.5
Carbon rage: 8-16

alkanes

Iso-alkanes

Cyclo-alkanes
Aromatics

Fractionation

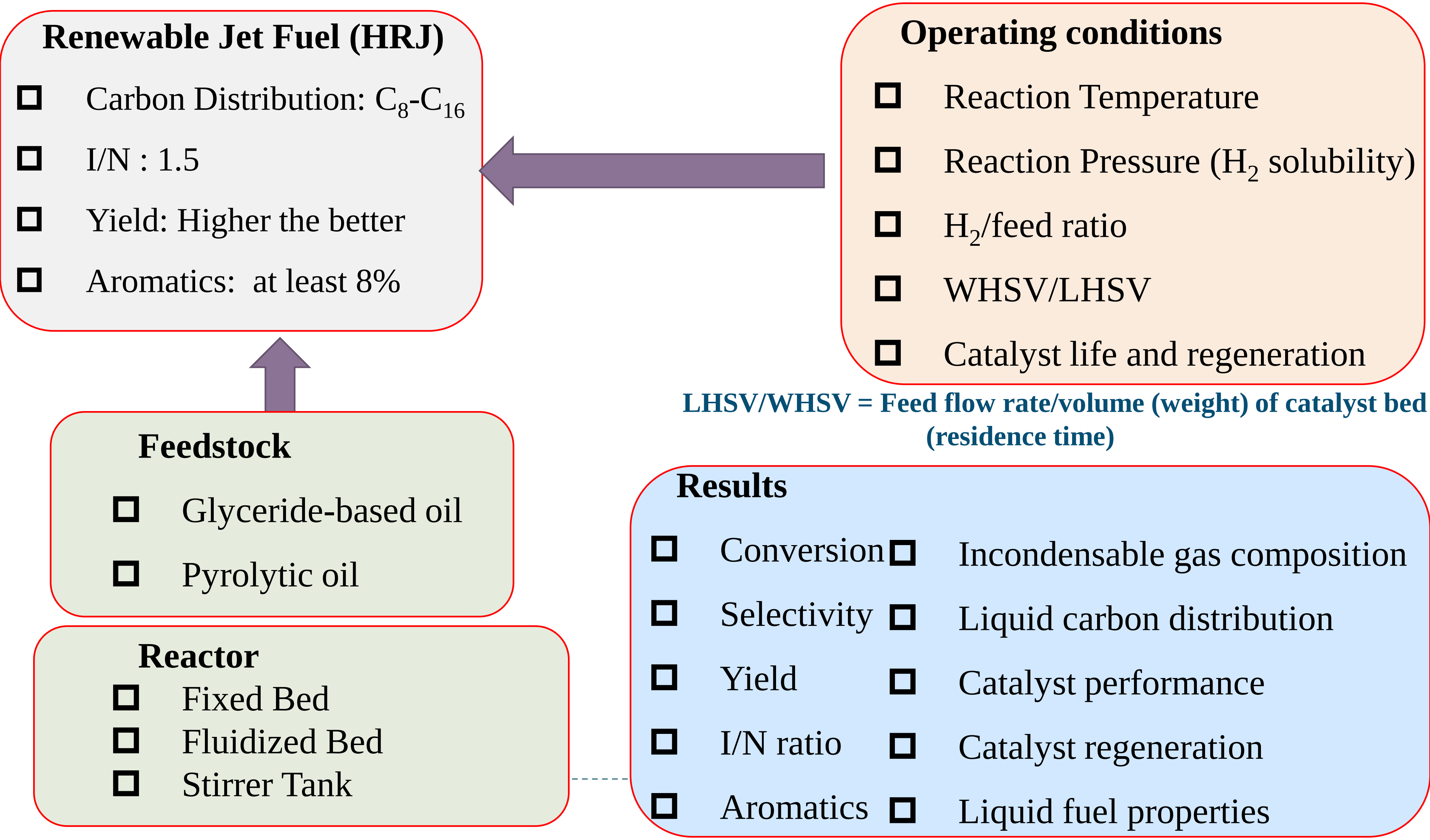
Light gases

Naptha

Jet (HRJ)

Diesel (HRD)

Renewable Jet Fuels



Renewable Jet Fuel (HRJ)

- ☐ Carbon Distribution: C_8-C_{16}
- ☐ I/N : 1.5
- ☐ Yield: Higher the better
- ☐ Aromatics: at least 8%

Operating conditions

- ☐ Reaction Temperature
- ☐ Reaction Pressure (H_2 solubility)
- ☐ H_2/feed ratio
- ☐ WHSV/LHSV
- ☐ Catalyst life and regeneration

LHSV/WHSV = Feed flow rate/volume (weight) of catalyst bed (residence time)

Feedstock

- ☐ Glyceride-based oil
- ☐ Pyrolytic oil

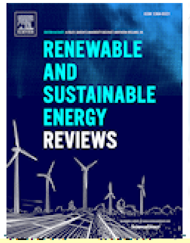
Reactor

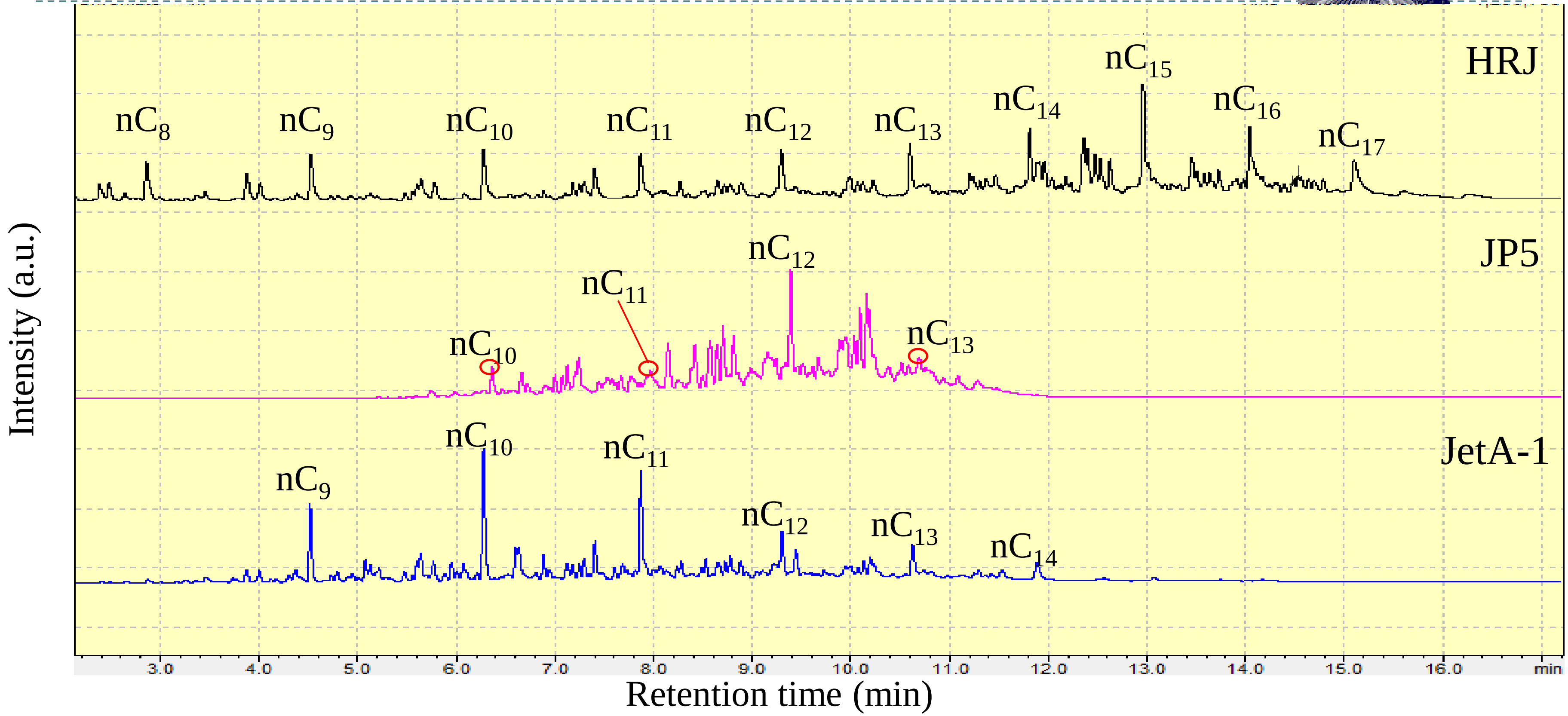
- ☐ Fixed Bed
- ☐ Fluidized Bed
- ☐ Stirrer Tank

Results

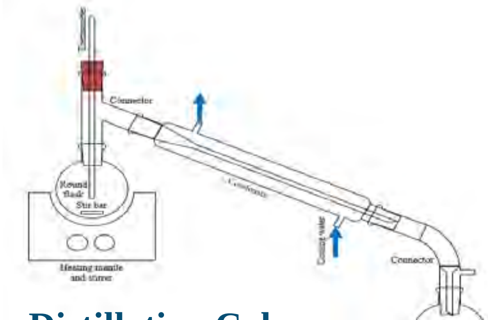
- ☐ Conversion
- ☐ Selectivity
- ☐ Yield
- ☐ I/N ratio
- ☐ Aromatics
- ☐ Incondensable gas composition
- ☐ Liquid carbon distribution
- ☐ Catalyst performance
- ☐ Catalyst regeneration
- ☐ Liquid fuel properties

Renewable Jet Fuels



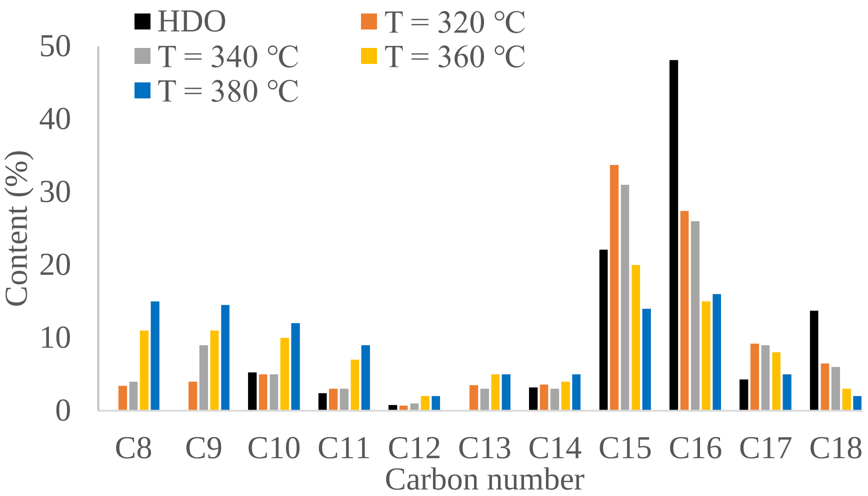


- JP-5 focuses on C_{10}-C_{13}，Jet A-1 focuses on C_9-C_{14}
- Need isomerize and crack the deoxygenated alkanes
- Can distillate the lighter and heavier products and concentrate the product in the target carbon chain

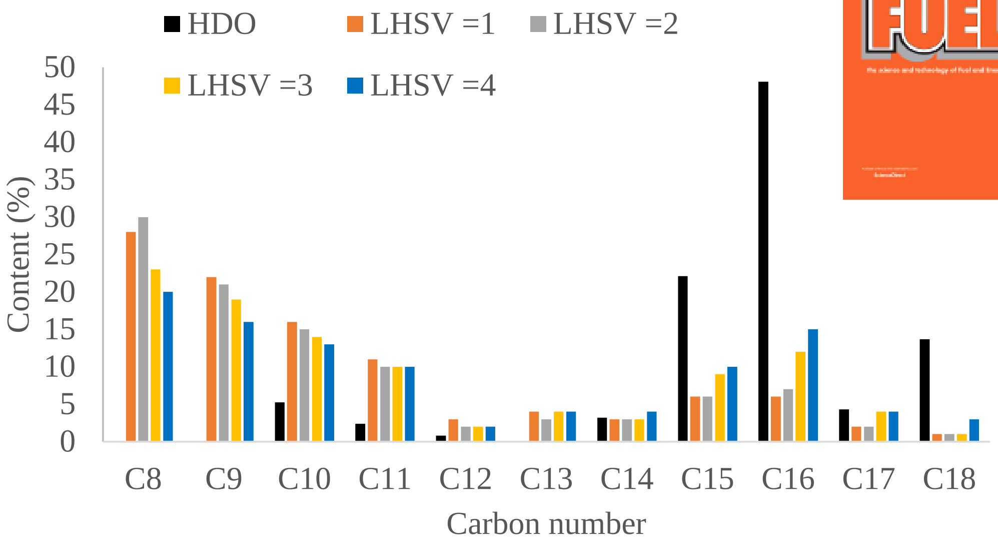


Distillation Column

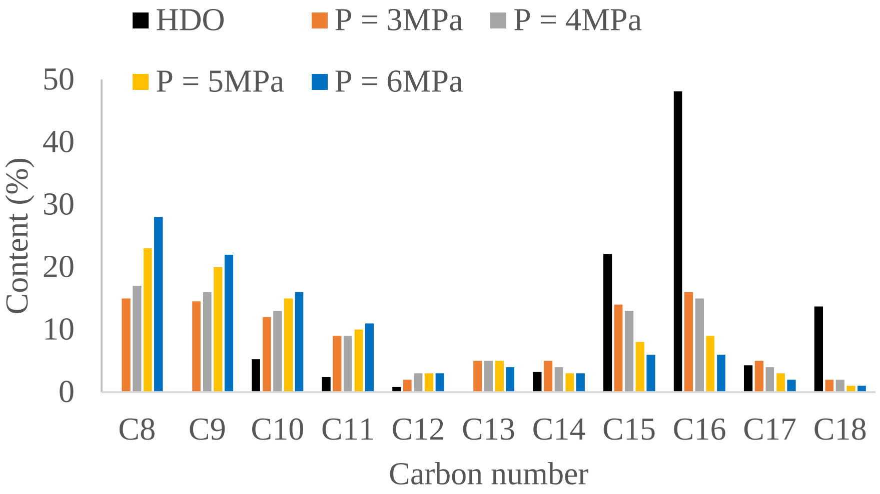
Feedstock: Glyceride-based Oil (carbon distribution)



Various Temperature



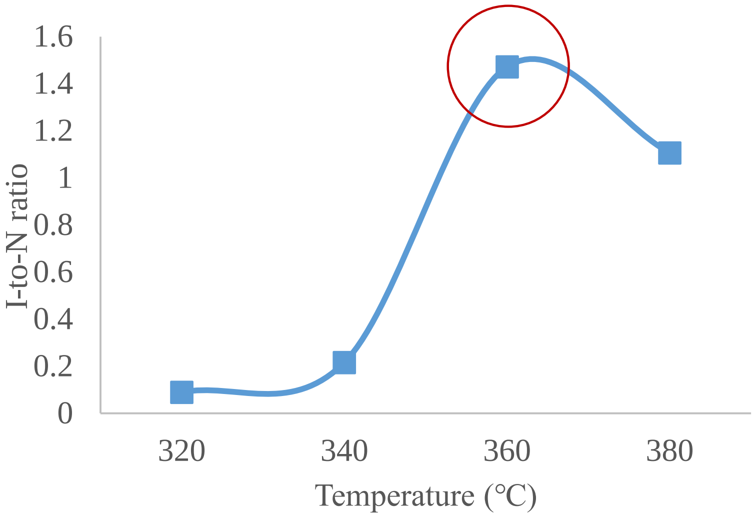
Various LHSV

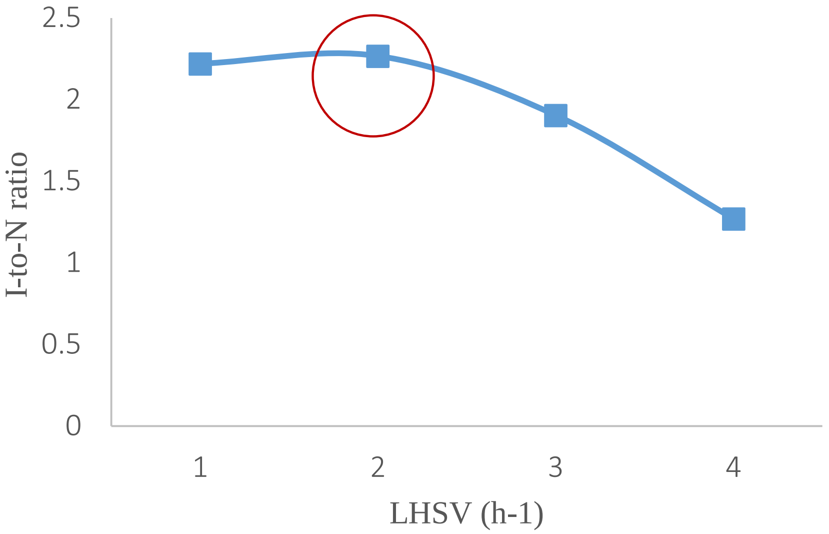


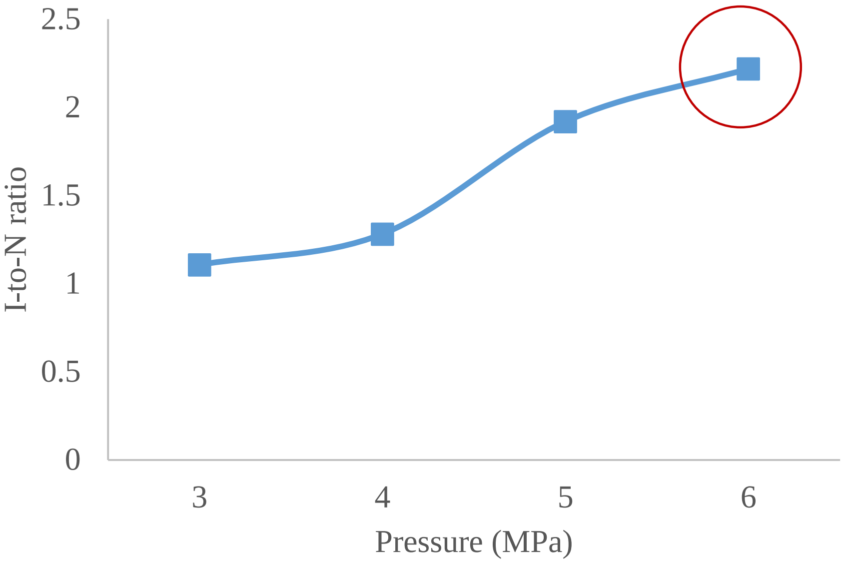
Various Pressure

- Feedstock: deoxygenated alkanes from palm oil
- Isomerization is slight exothermic reaction; cracking is endothermic reaction: cracking is more sensitive to the temperature
- Cracking starts from middle range carbon, the product concentrates on C_8-C_9
- High pressure favors cracking
- LHSV increases，shorter residence time，cracking decreases

Feedstock: Glyceride-based Oil (I-to-N ratio)

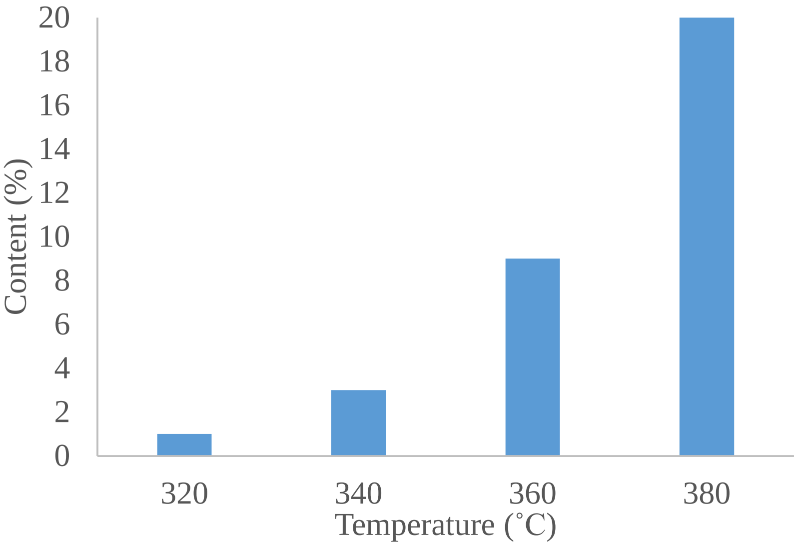


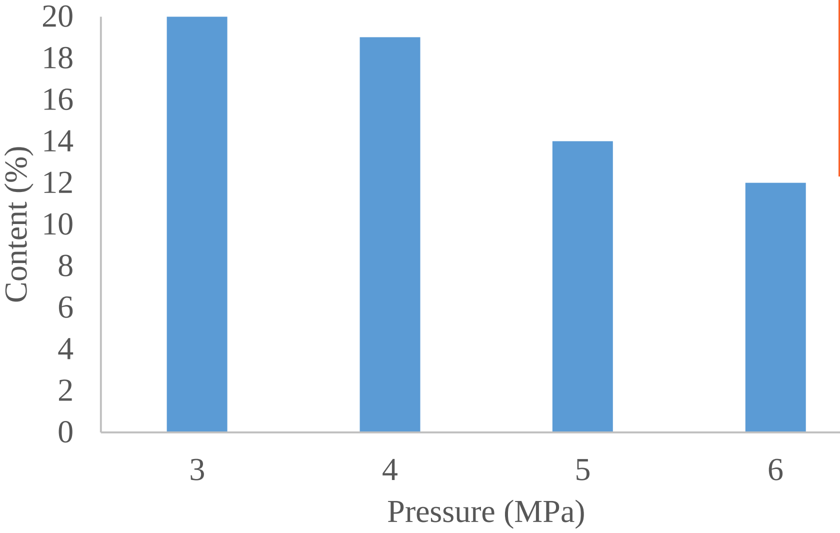


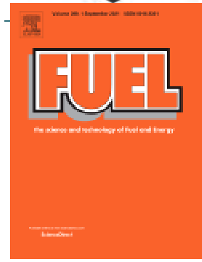


- At certain temperature，the amount of isomers is similar to traditional jet fuel
- High pressure favors isomerization
- Low LHSV promotes surface reaction and enhances the isomerization

Feedstock: Glyceride-based Oil -aromatics content



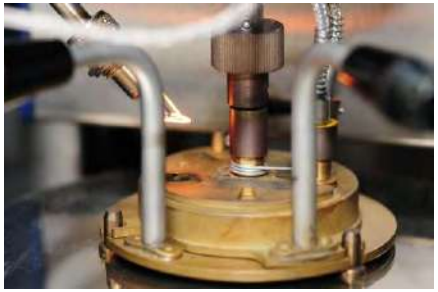



FUEL

- Producing aromatics needs dehydrogenation, which is favored by high temp and low pressure
- High pressure pushes aromatization reaction toward isomerization
- Aromatic content in jet fuel requires 8 %, based on ASTM D7566 Specification

Fuel Combustion Study


Laboratory development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Daily Use

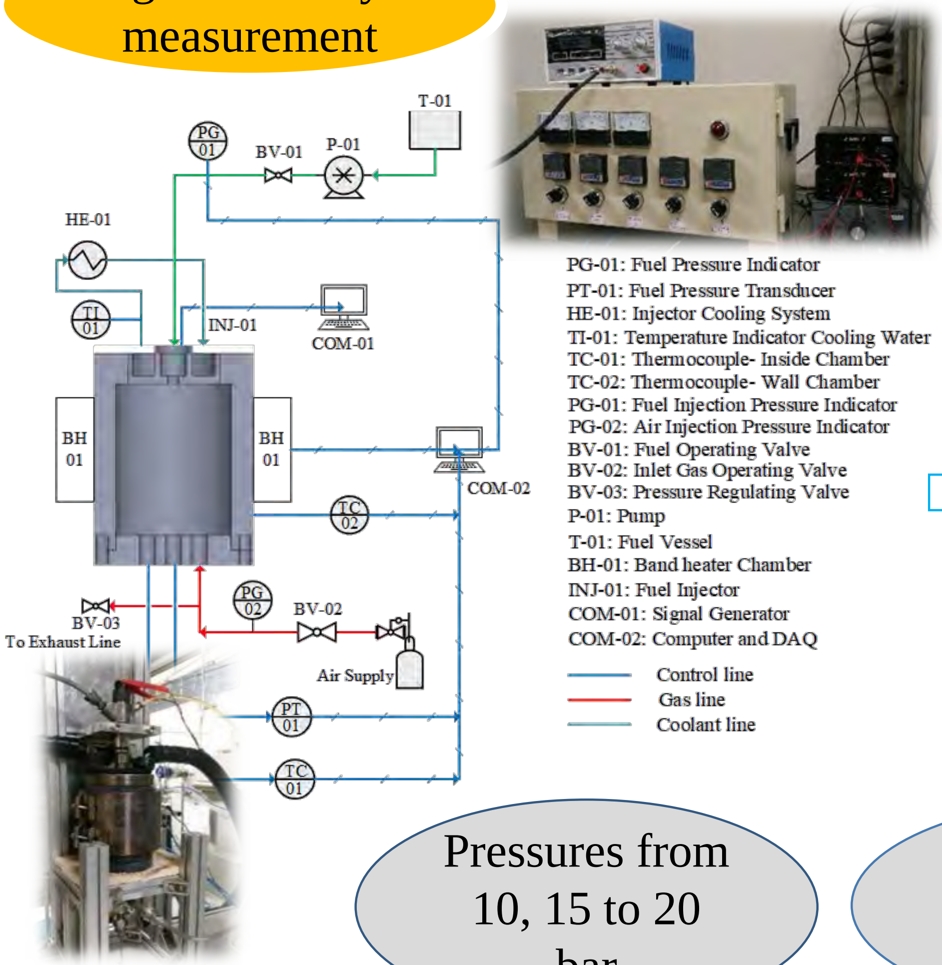
Ignition Delay

Ignition Delay Measurement-Constant Volume Combustion Chamber

The fuels

- HRD
- Biodiesel
- Diesel
- HRJ
- JP-5
- Jet-A1

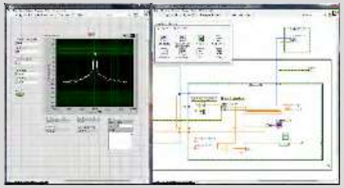
Ignition delay measurement



Pressures from 10, 15 to 20 bar

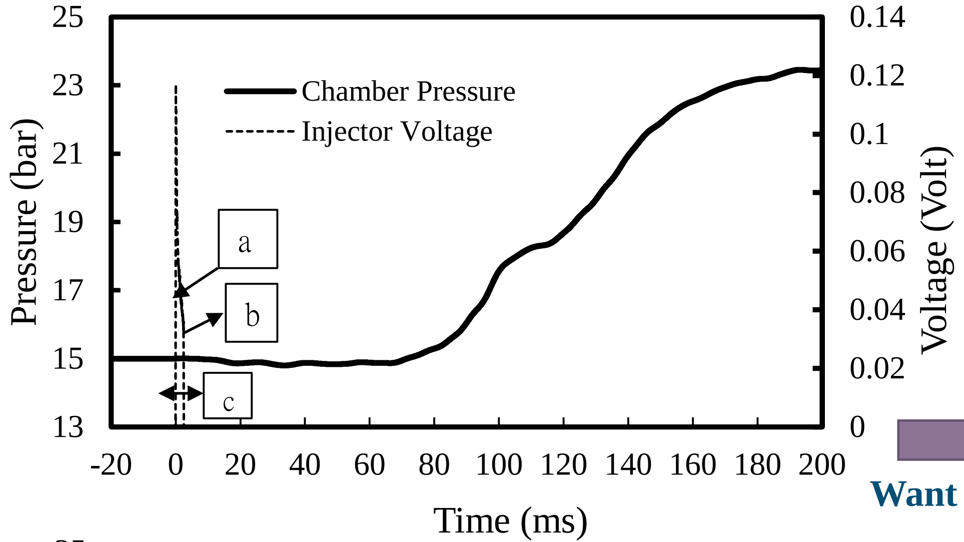
Temperatures ranging from 600 K to 818 K

Ignition delay analysis



LabView

Ignition Delay Measurement



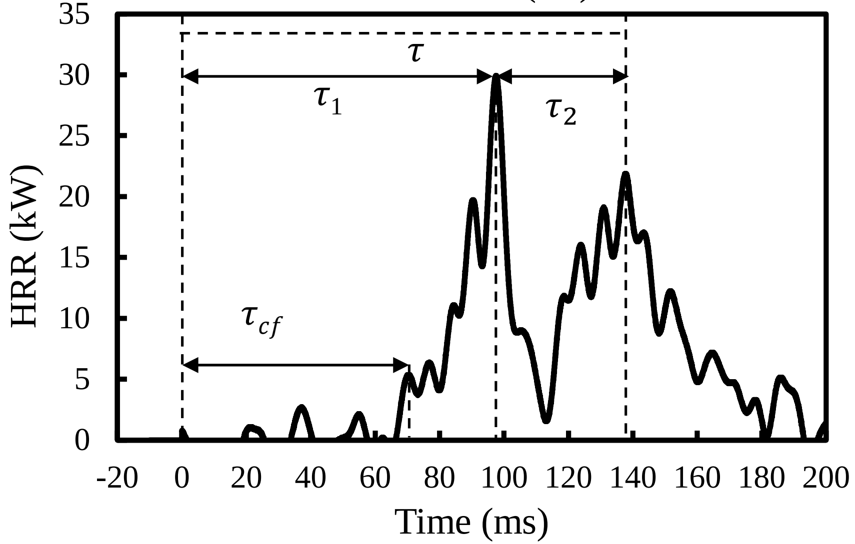
(a). Start of injection
(b). End of injection
(c). Injection duration

Want to look at

(1) (τ_{cf}). Cool-flame ignition delay
(2) (τ, τ_1, τ_2). Ignition delay
(3) HRR Curve
(4) Negative Temperature Coefficient

With Various

(a). Chamber Pressure
(b). Temperature
(c). Fuel



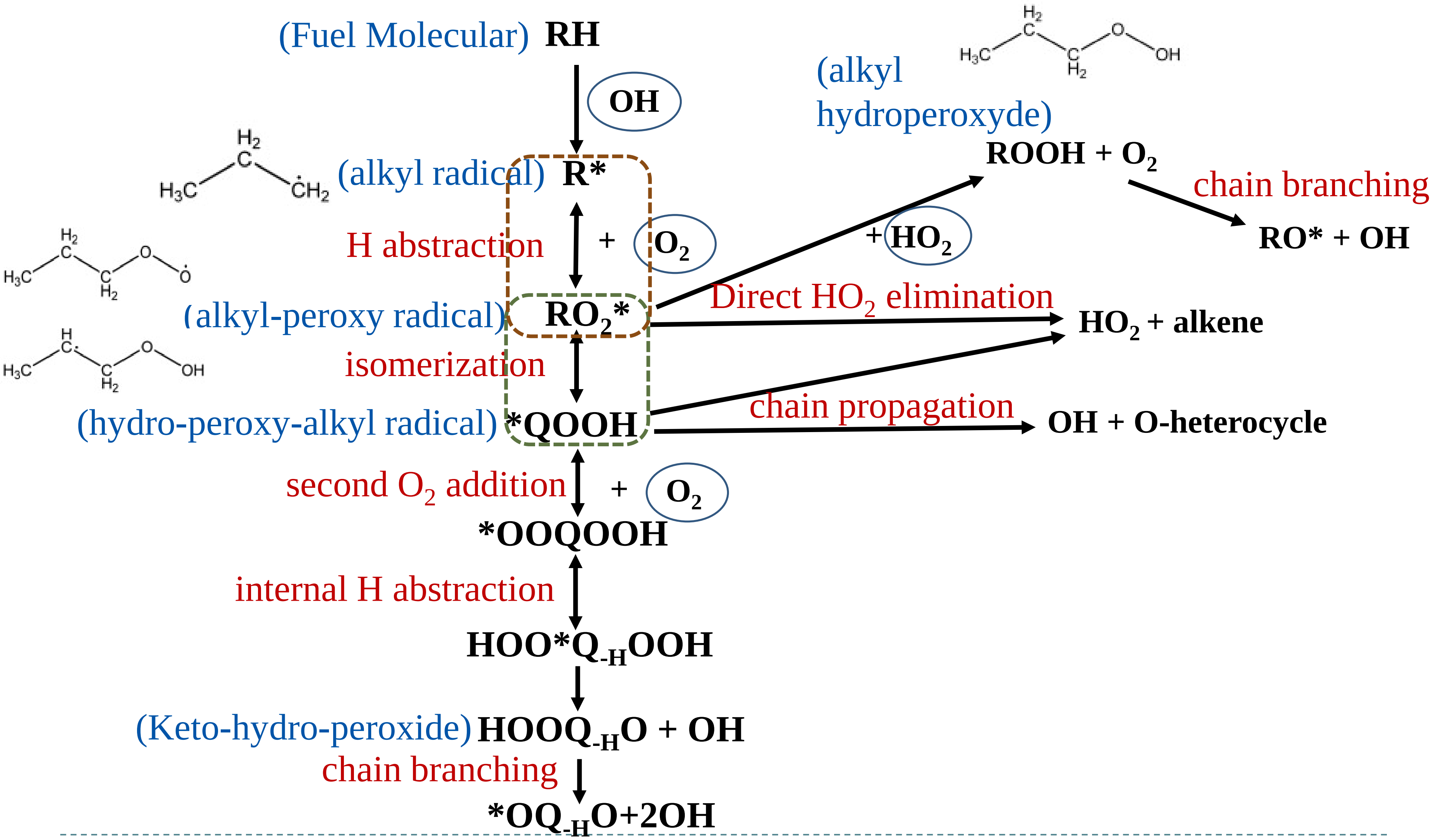
(τ_{cf}). Cool-flame ignition delay
(τ_1). First stage ignition delay
(τ_2). Second stage ignition delay
(τ). Total ignition delay

Heat Release Rate: $HRR = \frac{dP}{dt} * \frac{V_o}{\gamma - 1}$

Fuel: Jet A-1
T: 625 K ; P: 15 bar

V_0 & P : chamber volume and pressure
γ: specific heat ratio of the oxidizer

Low Temperature auto-ignition mechanism



(Fuel Molecular) **RH**

OH

(alkyl radical) **R***

H abstraction + **O_2**

(alkyl-peroxy radical) **RO_2***

isomerization

(hydro-peroxy-alkyl radical) ***QOOH**

second O_2 addition + **O_2**

***OOQOOH**

internal H abstraction

HOO*Q_{-H}OOH

(Keto-hydro-peroxide) **HOOQ_{-H}O + OH**

chain branching

***OQ_{-H}O+2OH**

(alkyl hydroperoxyde)

+ **HO_2**

ROOH + O_2

chain branching

RO* + OH

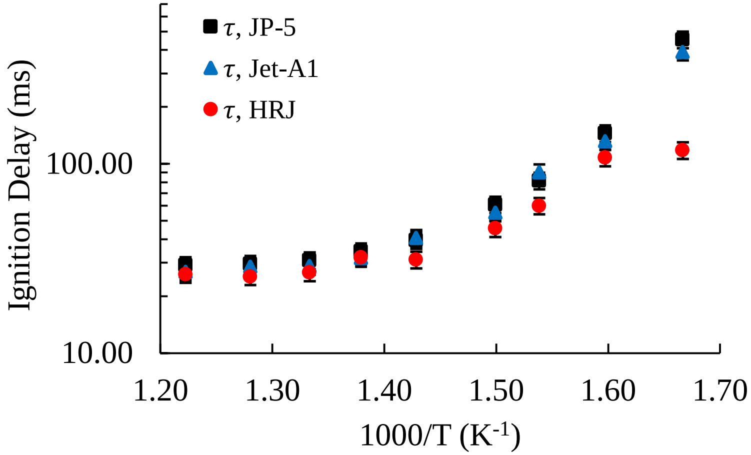
Direct HO_2 elimination

HO_2 + alkene

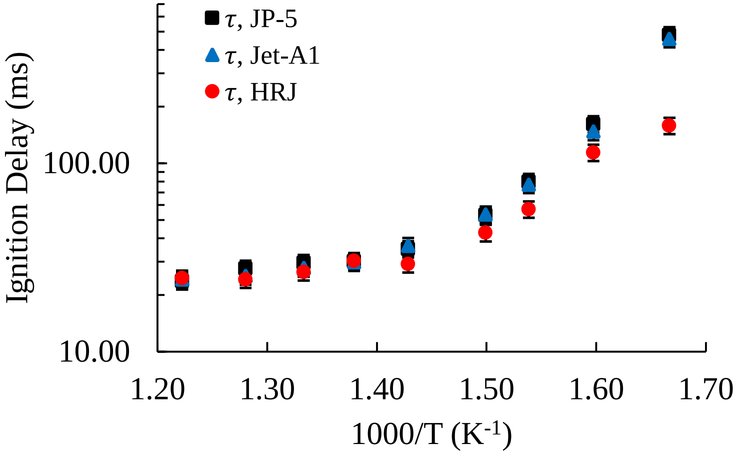
chain propagation

OH + O-heterocycle

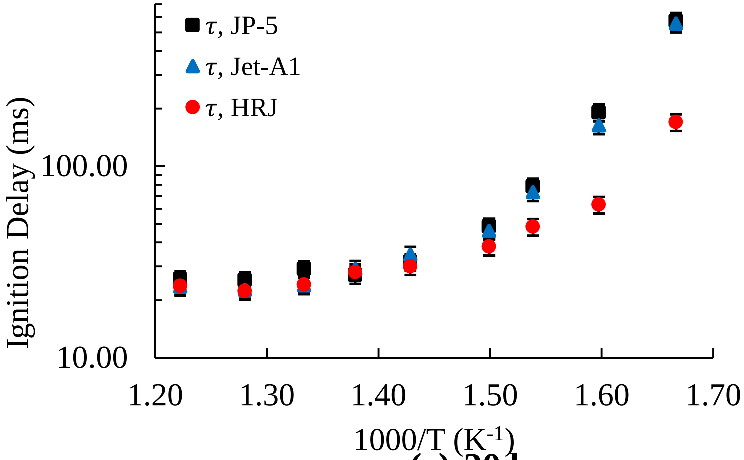
Total ignition delays – Jet fuels



(a) 10 bar



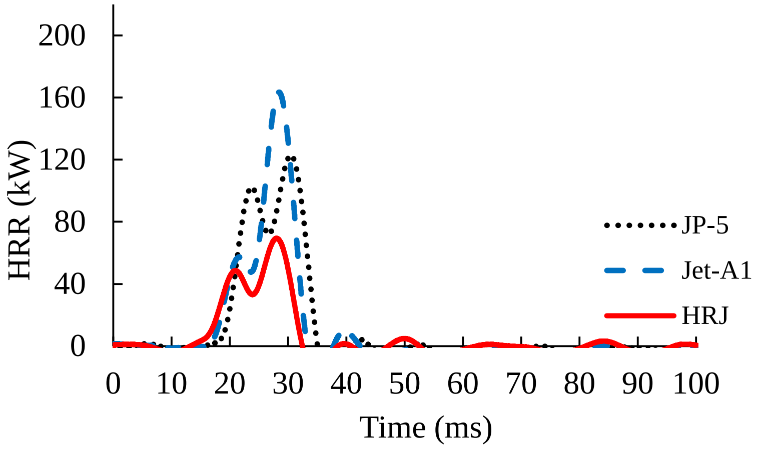
(b) 15 bar



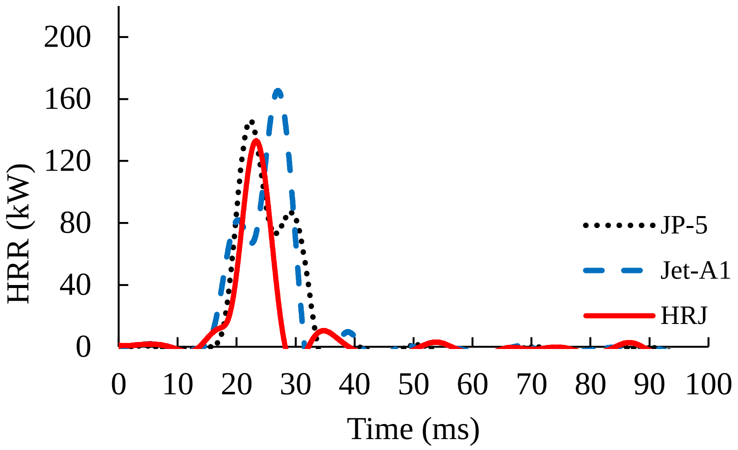
(c) 20 bar

1) Total ignition delay decreased with the increases in temperature
2) Ignition delay depends on H atom abstraction; $R+O_2 \leftrightarrow RO_2$ and isomerization; $RO_2 \leftrightarrow$ QOOH，the size of C-H bond influences the stability of H atom abstraction
3) Higher H/C, shorter ignition delay (HRJ)
4) Ignition delay: Jet A-1 shorter than JP-5 : Jet A-1 has 40 % more normal alkanes

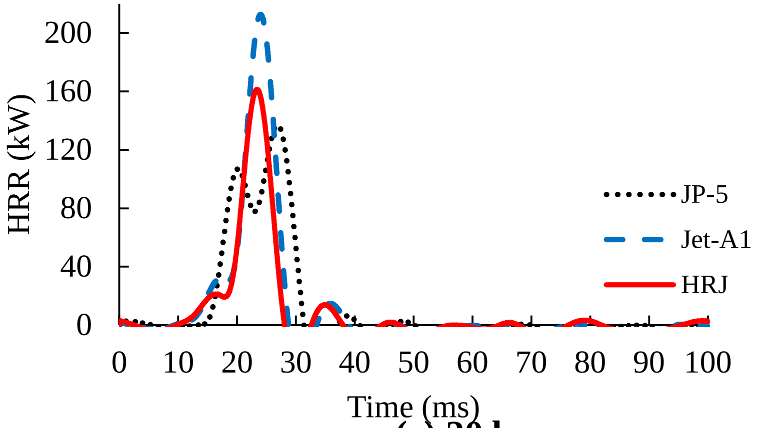
Heat release rate profile – Jet fuels



(a) 10bar



(b)15bar

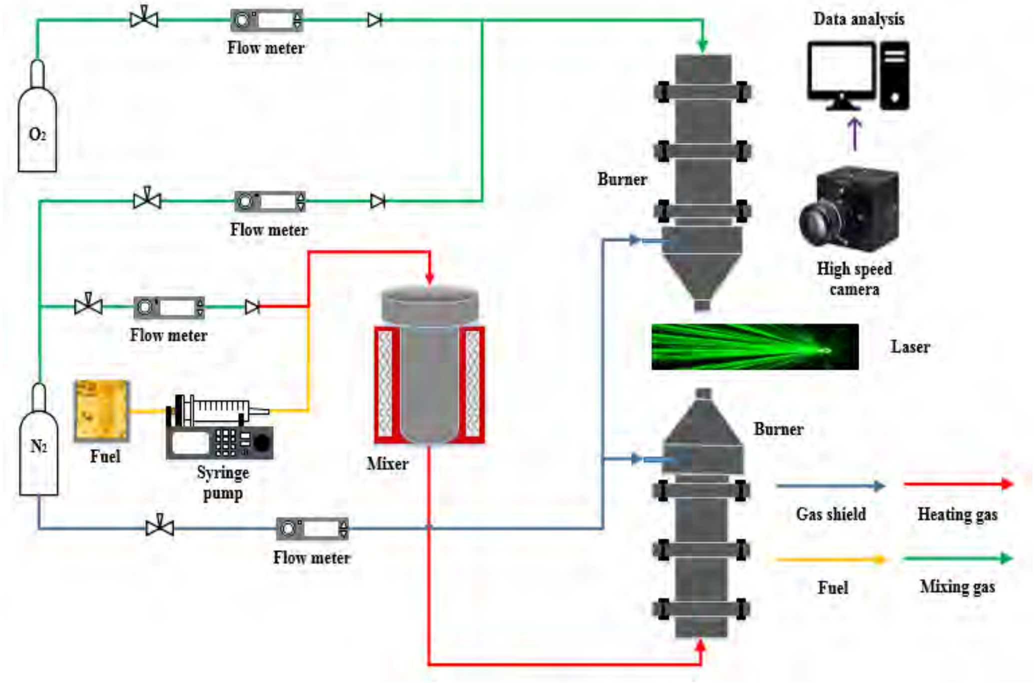


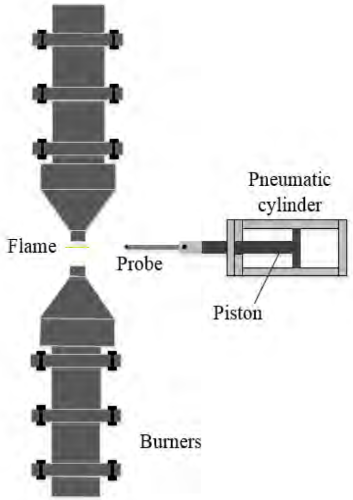
(c) 20 bar

1) The second peak comes from partial ignition due to non-uniform mixtures, more obvious at low pressure
2) The fuel with higher cyclo-alkane and aromatics has obvious two-stage ignition delay
3) The fuel with higher normal alkanes has little two-stage ignition delay

Soot Formation

Soot formation measurement





Thermophoretic sampling

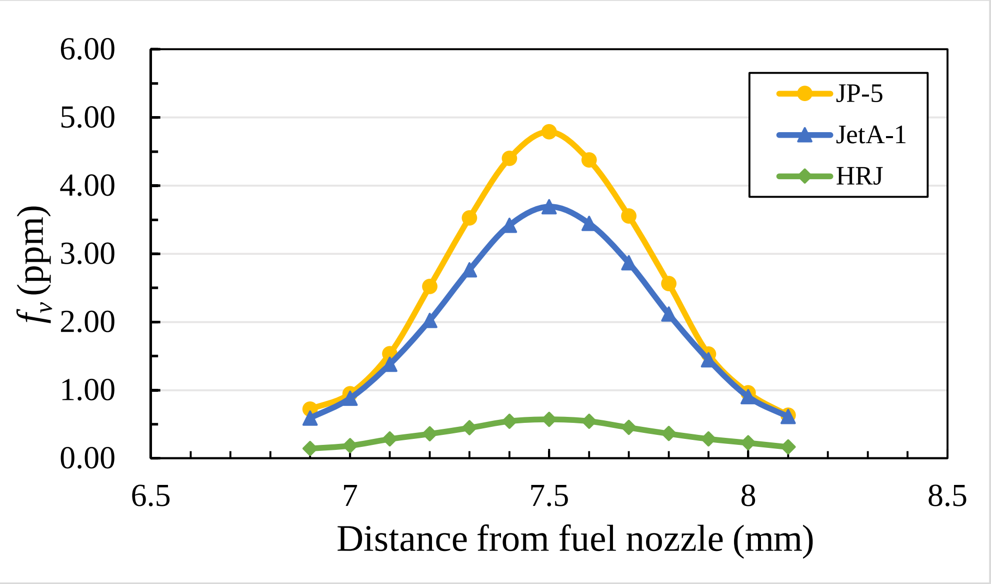
Smoke point tester

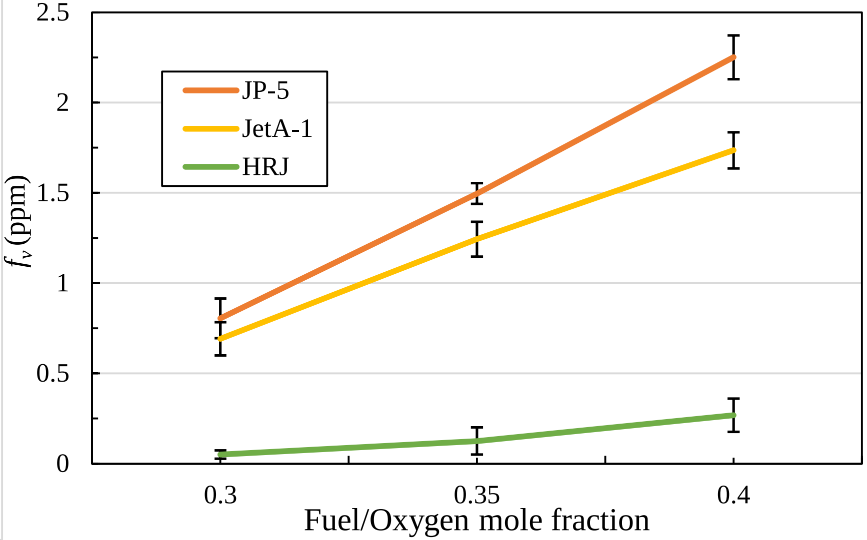
- LII(Laser-induced Incandescence) technique and counter-flow burner
- $\boldsymbol{f_v = \frac{\pi N D^3}{6}}$ and $\mathbf{N} = \boldsymbol{k_a}(\frac{A_a}{\pi d_p^2/4})^{\alpha}$ for soot volume fraction
- Using thermophoretic sampling and transmission electron microscopy
- Smoke point testing was carried out for verify the trend of soot volume fraction

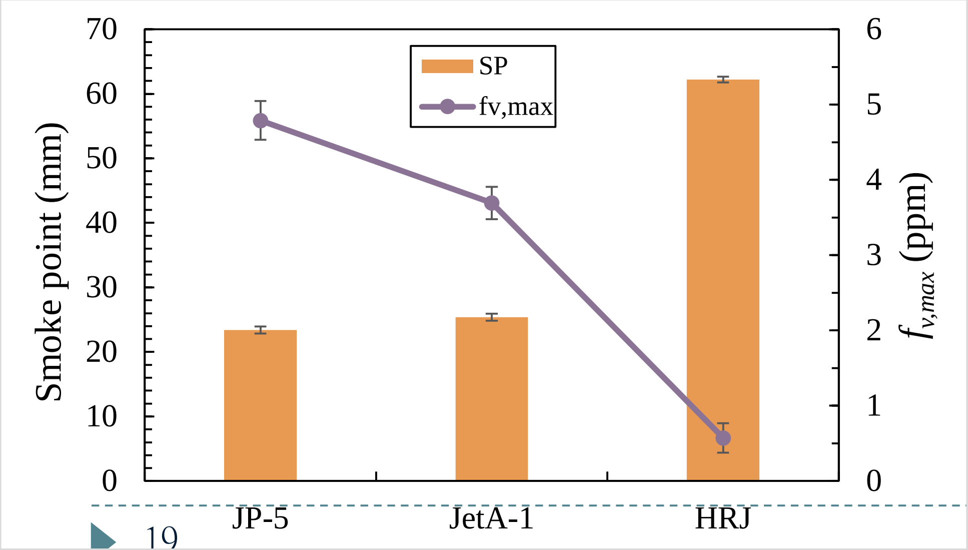
Transmission Electron Microscopy (TEM)

N : number of soot particles
D: average particle size
A_a : Area of LII signal

Soot formation for jet fuels

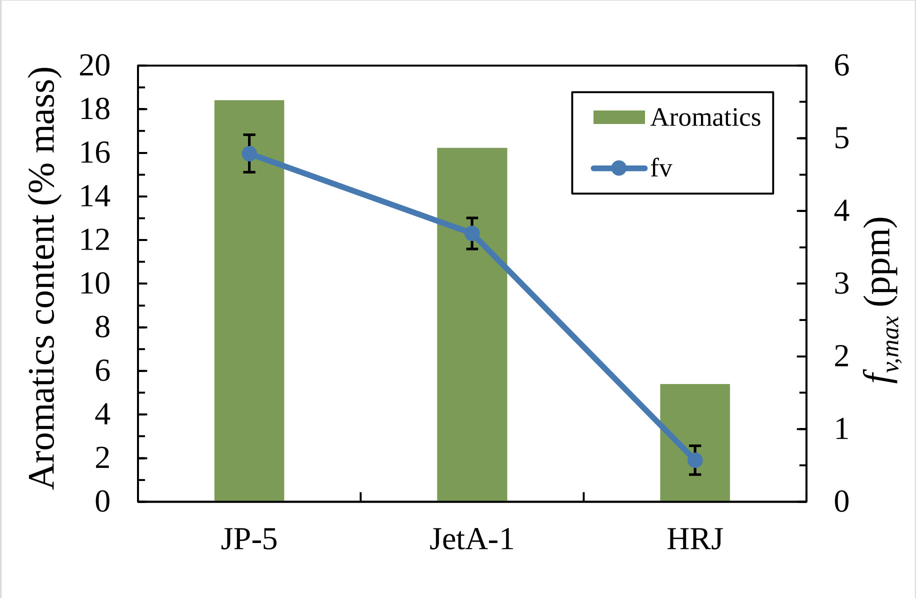


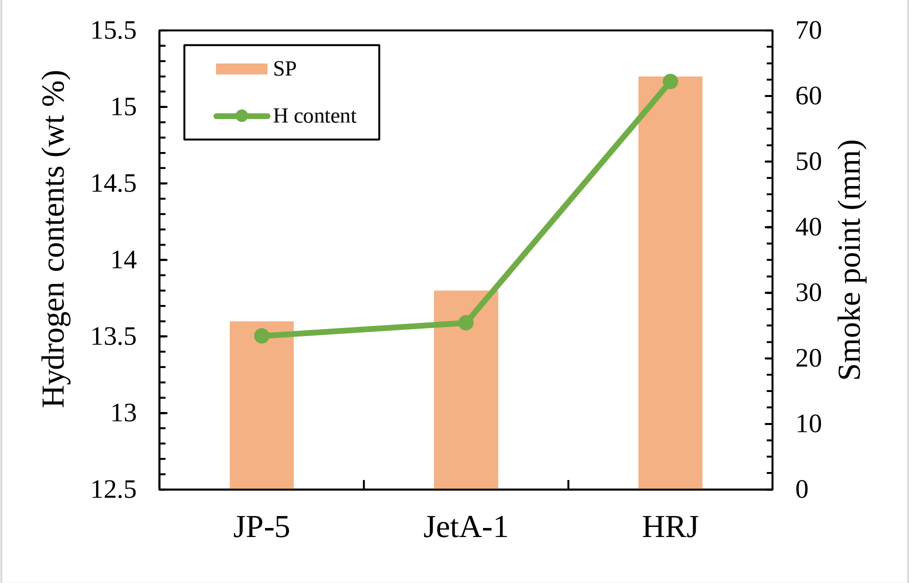




- ◆ Soot volume fraction of HRJ is the lowest (0.57 ppm), only 12 % of JP-5
- ◆ Soot volume fraction increases with increases in fuel fraction
- ◆ Smoke point: **JP-5 < Jet A-1 < HRJ** ， which verifies the measurement of soot volume fraction

Soot formation for jet fuels

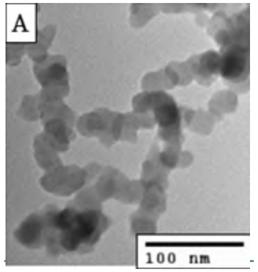




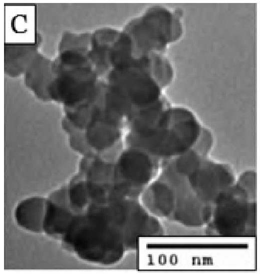
Composition(% mass)	JP-5	Jet A-1	HRJ
Aromatics (wt%)	18.4	16.2	5.4

- ☐ TEM: JP-5>Jet A-1> HRJ
- ☐ Higher H/C => lower Soot

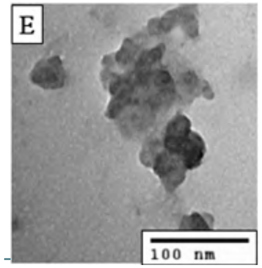
- ☐ The higher aromatics content, the higher soot
- ☐ Soot formation: normal alkane < isomer & cyclo-alkane
- ☐ Isomers => CH_2 & CH_3 radical，strengthen aromatics ring structure，deriving C_3H_3 radical，which forms PAH



JP-5



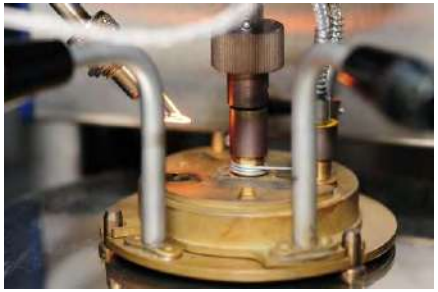
Jet A-1



HRJ

Process Evaluation

Laboratory development



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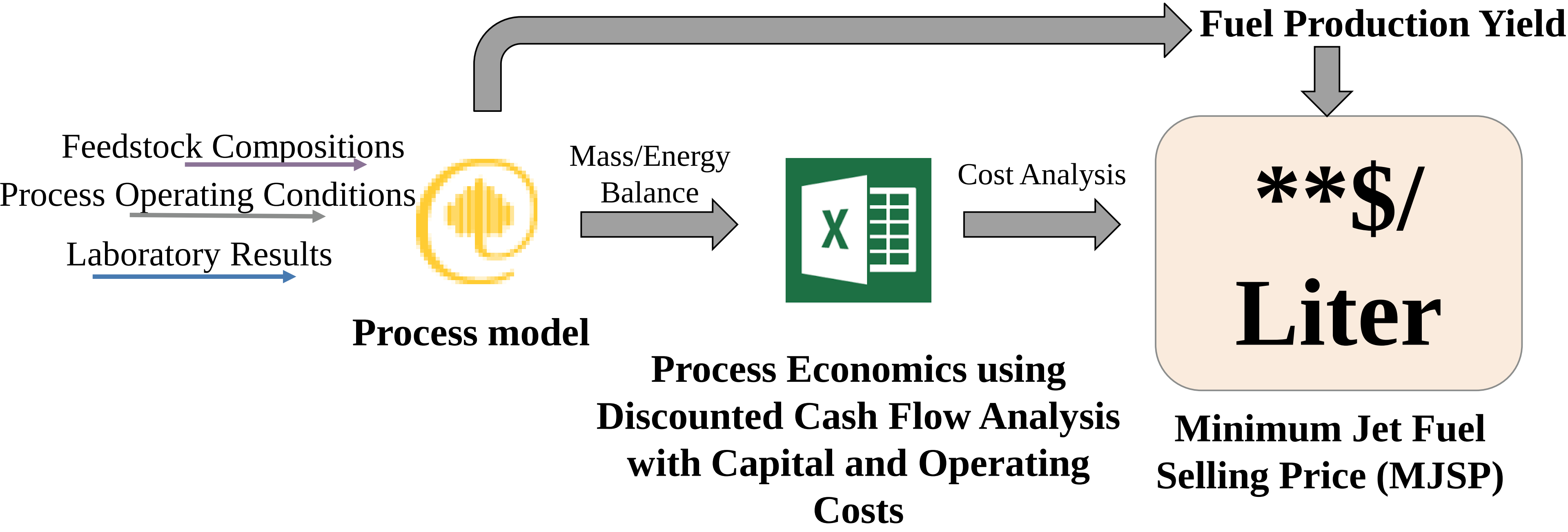


Feedstock Compositions

Process Operating Conditions

Laboratory Results

Process model

Mass/Energy Balance

Cost Analysis

Process Economics using Discounted Cash Flow Analysis with Capital and Operating Costs

Fuel Production Yield

****$/ Liter**

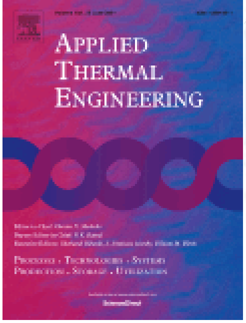
Minimum Jet Fuel Selling Price (MJSP)

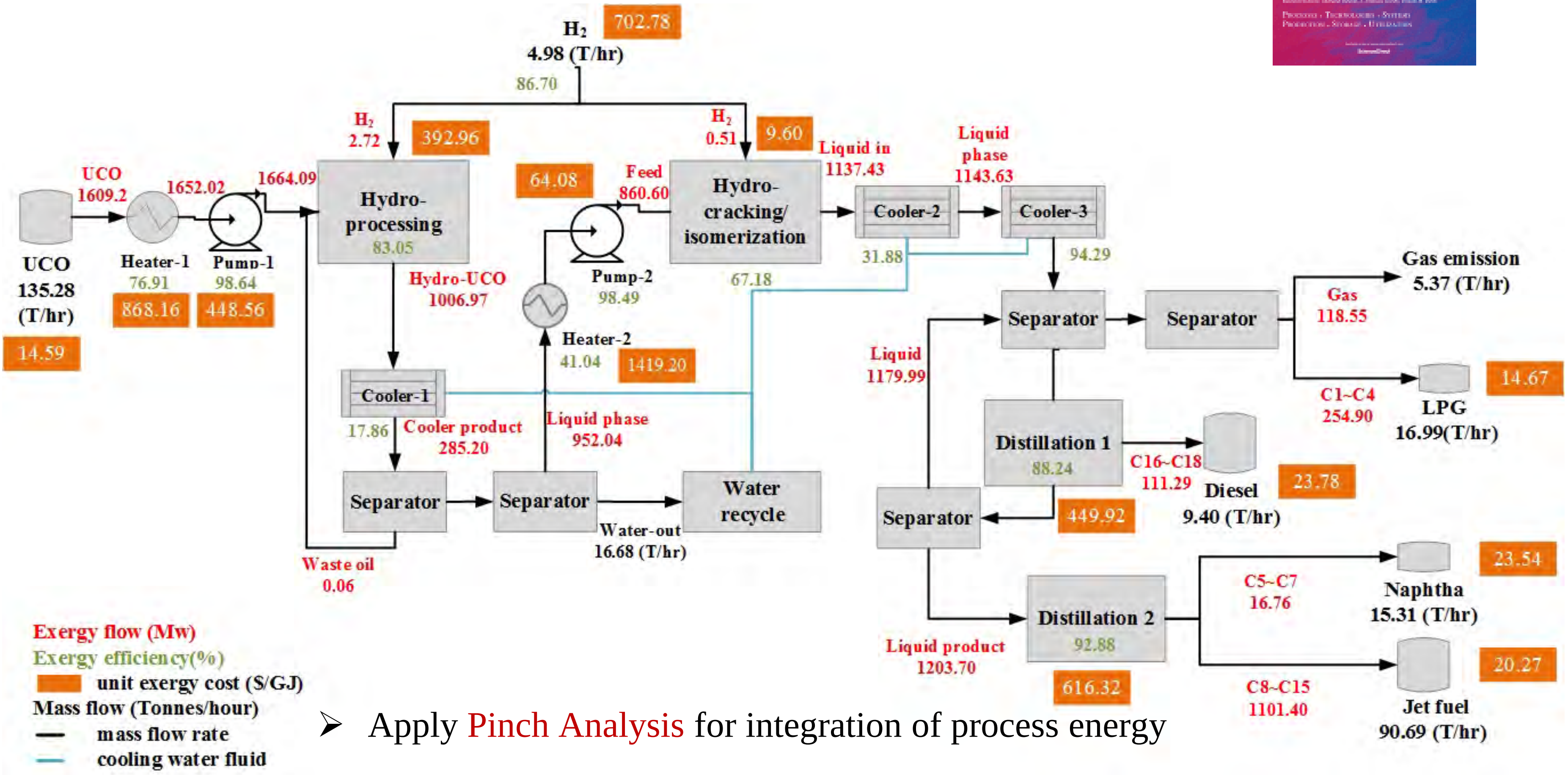
Process Evaluation

- ☐ Laboratory operating conditions
- ☐ Equipment quotation
- ☐ Local situation

- ☐ Mass/Energy/Carbon Flows
- ☐ Exergy/Pinch Analysis
- ☐ Techno-Economic Analysis
- ☐ 3E (Energy/Economic/Environment)

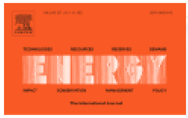
Process Evaluation (Mass/Energy/Exergy Flow)



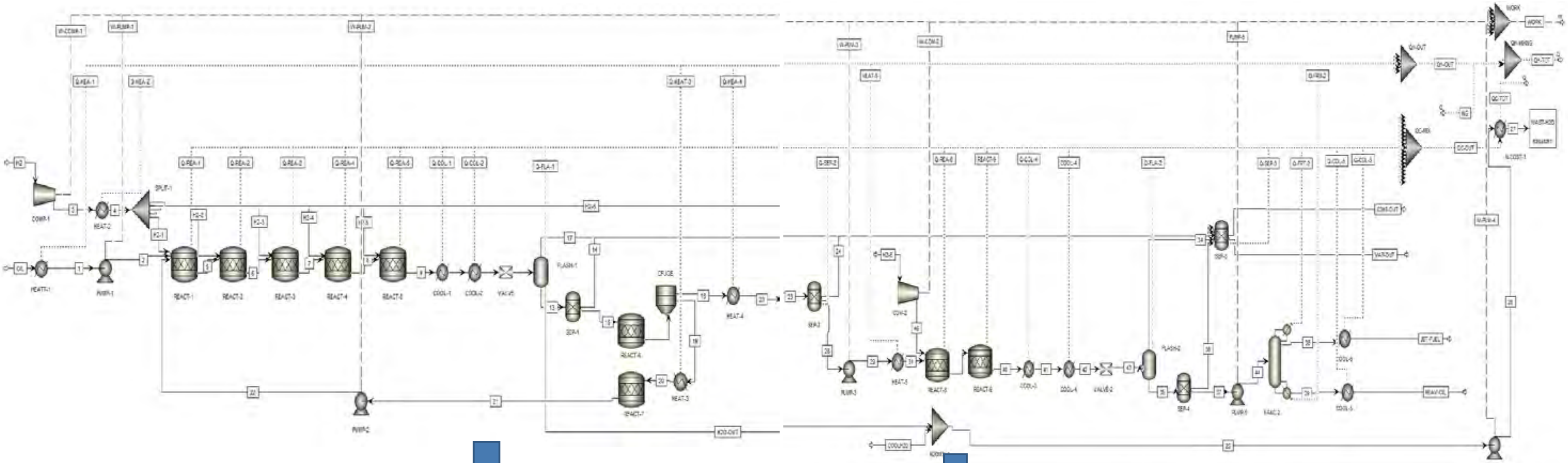


- ➢ Apply Pinch Analysis for integration of process energy
- ➢ Define system Exergy Destruction and combine Thermo-economic Analysis to find Cost of Exergy Destruction
- ➢ For large Exergy Destruction, apply Energy Integration (heat exchangers..etc) for maximizing the process energy efficiency

Process Evaluation
(Techno-Economic Analysis)



Process Simulation



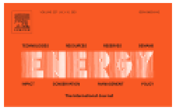
Vendor-quoted Capital Cost **Mass and Energy Flows** **Locally evaluated Operation Cost**

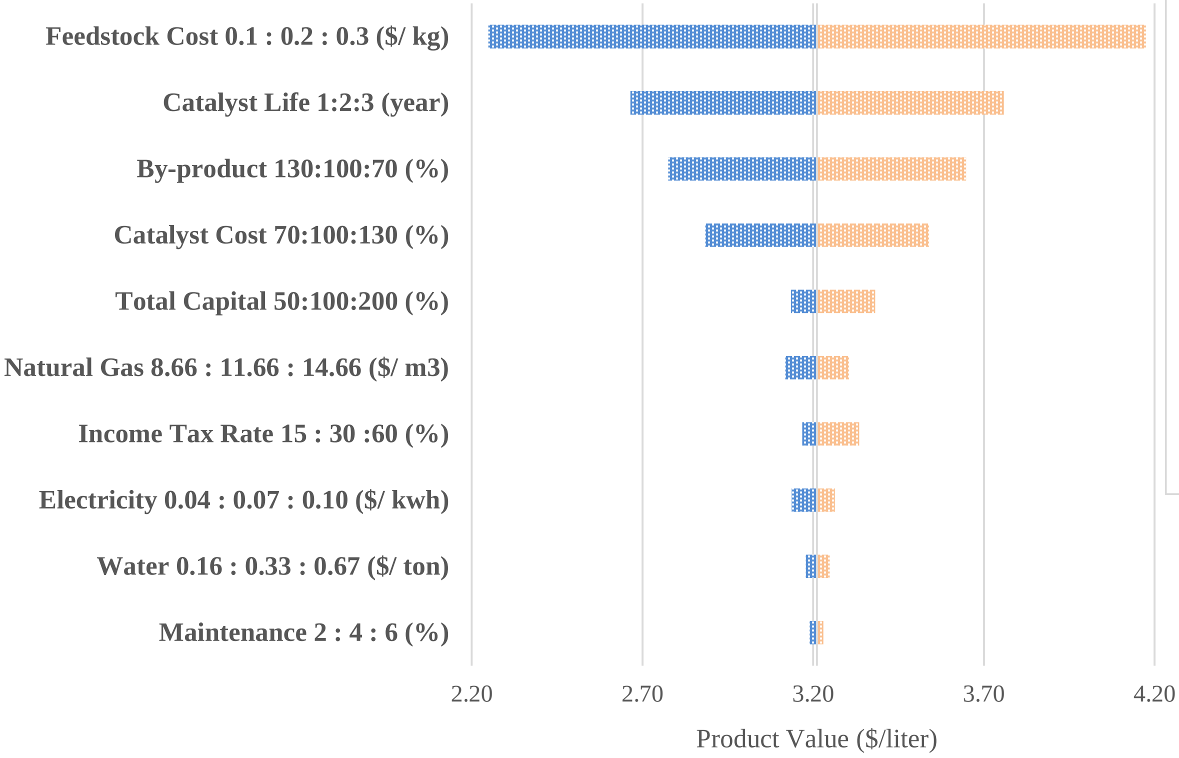
Plant Assumptions	
Basis Year for Analysis	2017
Plant Life	30 years
Plant Depreciation	8 years
Total Income Tax Rate	30%
Operating hours	8088 hours
Plant Capacity	600 tonnes/day
Feedstock Cost	original cost + shipping fee
Internal Rate of Return	10%
Prices of the catalyst	vendor quotation
Annual interest rate and term for financing	6 %, 5 years
Debt/equity for financing	60%
Price of the by-products	quotation

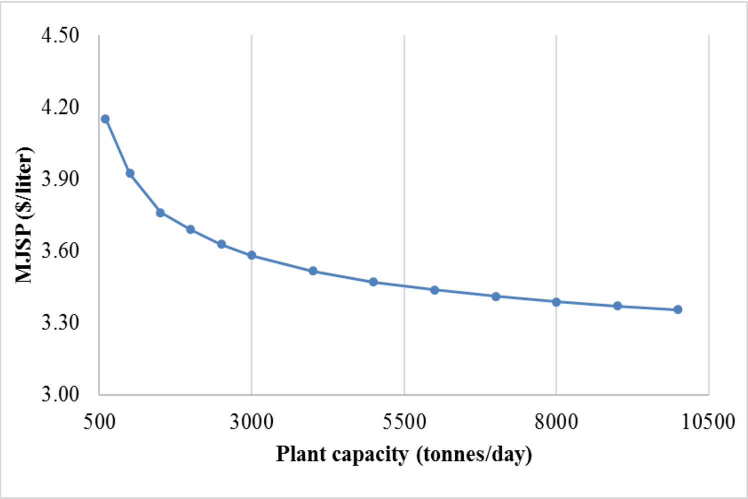
Mass/Energy/Carbon Balance
Techno-economic analysis(TEA)

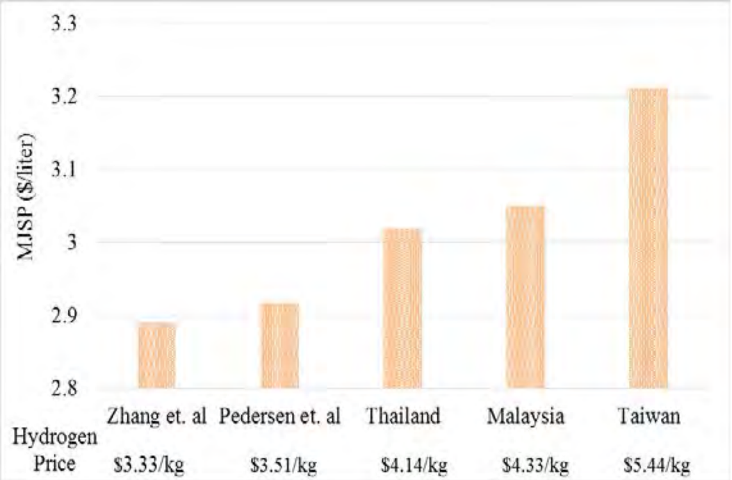
	Oil scenario
Capital cost (million $)	284
Operating cost (million $ per year)	134
Fuel yield (million gal per year)	29.8
MJSP ($/liter)	**1.43**
Co-product credit (million $ per year)	27

Process Evaluation (Sensitivity Analysis)



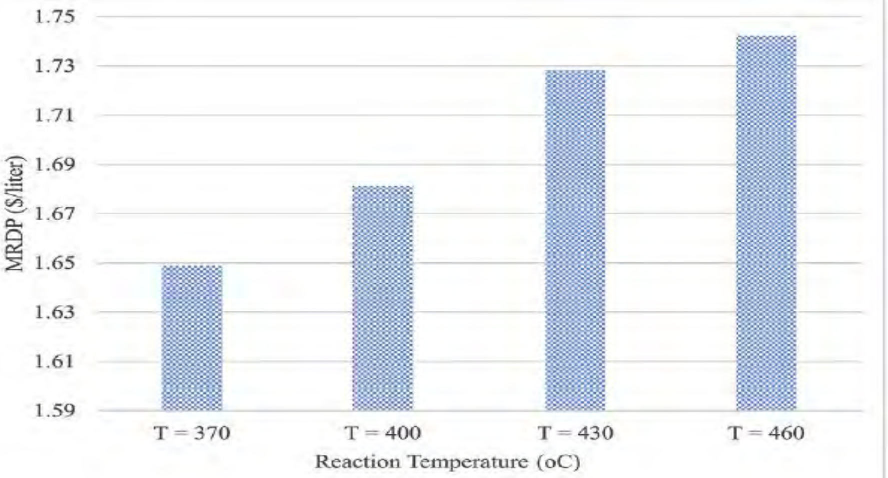




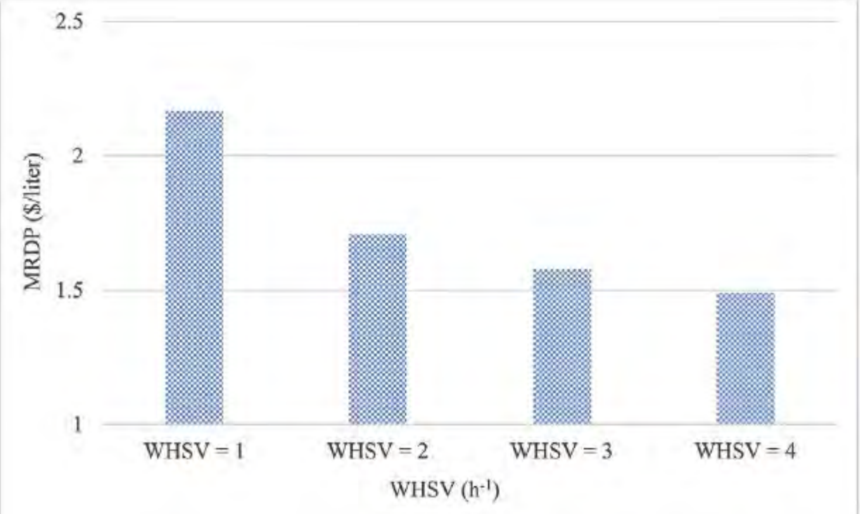


- Sensitivity Analysis points out feedstock is the most effective factor
- Increase capacity reduces MJSP, but only to a certain amount
- Fuel selling price increases with increasing hydrogen price

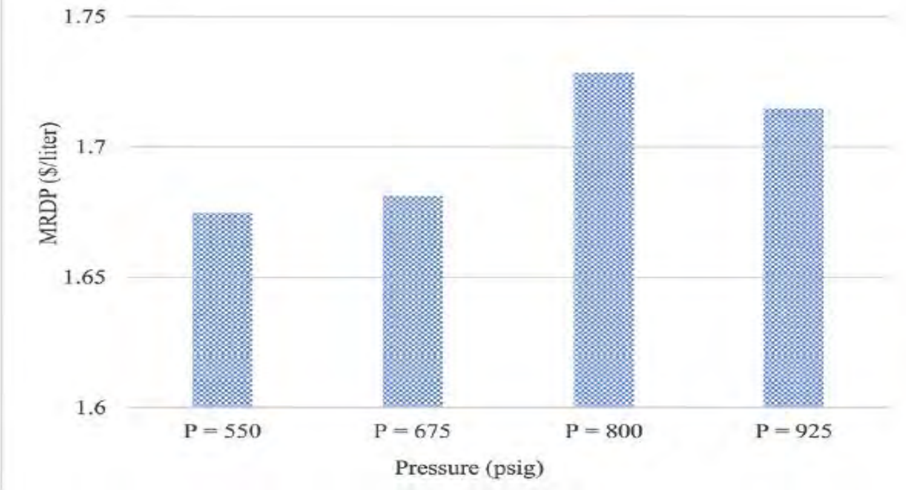
Process Evaluation
(Effects of operating condition)



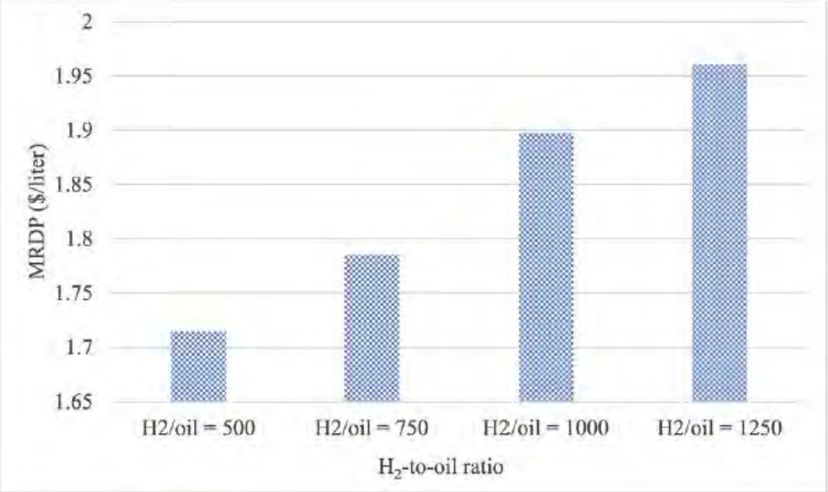
- **High temperature reduces the selectivity of the target product, and reduces the yield. Fuel price goes up**



- **Higher WHSV increases the fuel production yield per catalyst mass.**



- **High pressure increases the safety requirement of the system. Increase the CAPEX**

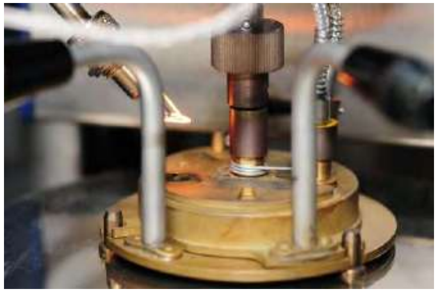


- **More hydrogen increases the production cost**

Conclusion-Now and the Future

Laboratory development

Novel Jet Fuel Development



Fuel Combustion Test

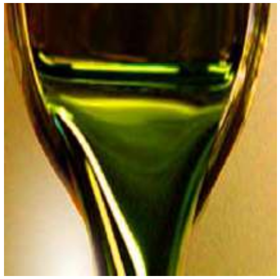
1. Ignition
2. Soot Formation

Process Evaluation

1. mass/energy/carbon balance
2. Exergy Analysis
3. Techno-economic Analysis

Current Study

Future Work



Feedstock Solution

Waste-to-Energy??
Waste-to-Fuel??

Transportation Test

Commercialization

Financial Support

Distribution pipeline

Daily Use

Government Support

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