Low-temperature Ignition of DME-air Mixture in A Straight Heated Tube Reactor

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Background – DME

Dimethyl ether (DME):

\[ \text{CH}_3\text{OCH}_3 \]

**DME: Multi-Use, Multi-Source Low Carbon Fuel**

- Transportation
- Cooking & Heating
- Power Generation

**Good ignition properties**

- Low soot formation
- Low NOx emission
- etc…

**Higher Reactivity at Low-temperature**

**Internal combustion engine design**

**Oxidation of DME at low-temperature should be better understood!**

**SAFETY FIRST!**

From IDA website
http://aboutdme.org/index.asp?sid=1
Background – cool flame region of DME

Pressure (atm)

Temperature (K)

Curran, (2000)
Low-T Part

Pfahl, (96)

Dagaut, (98)

Liu, (2001)

Curran, (98)
&Dagaut, (96)

Maruta, (2010)
Curran, 2000
High-T Part

Slowly peroxide oxidation >>> cool flame >>> NTC >>> high-T oxidation >>> explosion

Cool Flame?

Cool Flame

NTC zone

High-Temperature Oxidation and combustion zone

NTC zone

High-Temperature Oxidation and combustion zone
Low-temperature auto-ignition was captured in a specific temperature and ER range.
Objective

- What’s the effect of the “corner” in U-shape reactor used in previous study?
- What’s the mechanism of the observed low-temperature auto-ignition?
- Why does the auto-ignition occur in the specific narrow range?
The auto-ignition is due to the chemical nature of DME, but not the irregular shape of the previous U-shape reactor.
Results – Periodic hot flame ignition

Flow rate of mixture: 78 ml/min    Equivalence ratio: 1.47    Exposure time at 900 mm: 48 s

Periodic “cycle” behavior with robust periodic duration

Estimated flame propagation speed by image is higher than 0.88 m/s.
Results – Periodic two-stage ignition

Flow rate of mixture: 78 ml/min  
Equivalence ratio: 1.73  
Exposure time at 900 mm: 48 s

Temperature at 400 mm from inlet  
Temperature at 900 mm from inlet

Weak flame  
Hot flame

Both flames propagate!

One cycle = multiple weak flames + one hot flame
Results – Gas analysis

Time sequential gas analysis

- t1: 50 seconds after hot flame
- t2: 15 seconds after the first weak flame
- t3: 15 seconds after the last weak flame
- t4: 10 seconds after hot flame

Stable Oxidation: DME, O2 → HCHO, HCOOH, CH3OCHO

Chain-propagation reactions:

Ignition: DME, O2 → CH4, C2H2

Chain-branching reactions:

Results at 400 mm

Results at 900 mm
Discussion – Possible chain-branching steps

The auto-ignition may due to the accumulation of these peroxides and hydroperoxides.

The self-inhibition behavior may due to the thermal decomposition of these peroxides and hydroperoxides on account of sudden rising temperature.
Discussion – Controversy on HPMF in DME oxidation

HPMF (HOOCH$_2$OCHO), which was proposed by Curran DME-2000 Mechanism, has never been confirmed in any experiment so far.

HPMF (HOOCH$_2$OCHO) 

chain branching 

HCO + HCOOH 

H$_2$O + HCOO COH 

HOOCH$_2$OCH 

*CH$_2$OO* + HCOOH 

H$_2$ + CO + HC = OOOH 

... 

HPMF may lead some new propagation pathways; Also, there may be other chain-branching pathways exist without passing through HPMF.

High temperature dependency of the ignition

Improvement on the chain-branching steps of DME oxidation mechanism is necessary!
Conclusions

- Two kinds of flames (weak and hot) in DME/air mixture were captured with a constant equivalence ratio and temperature;

- The auto-ignition should be induced by the chain-branching precursors, CH$_2$OCH$_2$OOH and other possible peroxides and hydroperoxides, which may accumulate in a relatively longer exposure time;

- CH$_4$ and C$_2$H$_2$ act as two kinds of species due to the low-temperature ignition. Formation of HCHO, HCOOH, and CH$_3$OCHO are mainly due to stable oxidation;

- The ambiguity of reactions related to HPMF can be one of the important reasons that causes the strong temperature dependency of the auto-ignition.
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