# The Effect of Dimethyl Ether Addition on Sooting Limits in Counterflow Diffusion Flames at Elevated Pressures

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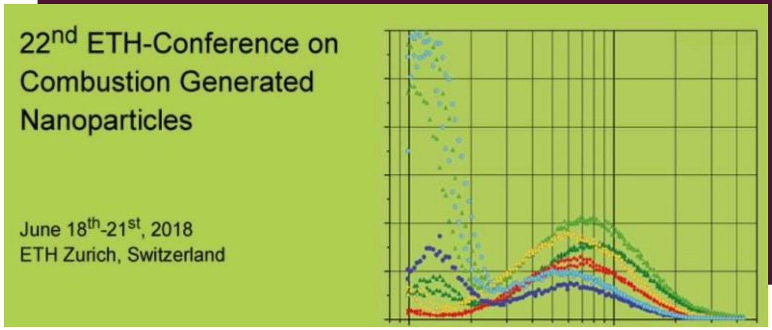


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- Results and Discussion
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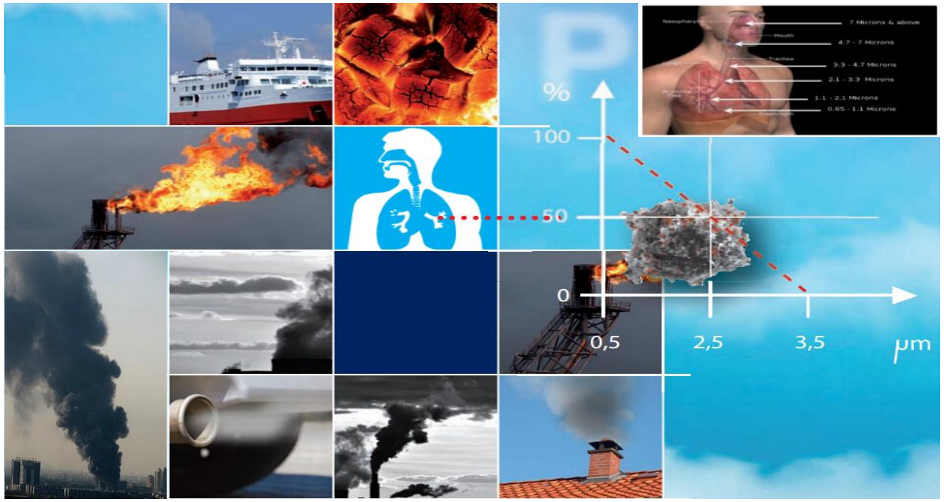
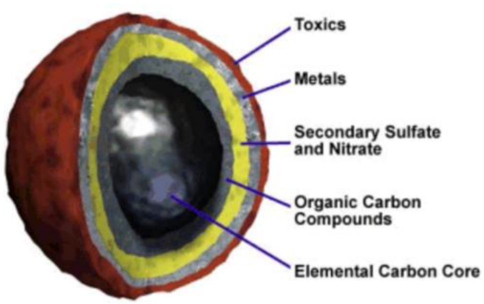
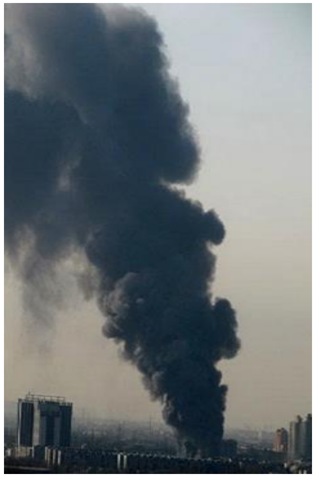


# Motivation and background

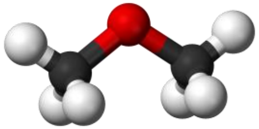
**Soot**: carbonaceous particles resulting from incomplete combustion of hydrocarbon fuels.



- Incomplete Combustion: Efficiency
- Deposition : Burner Lifetime / Performance
- Health: Carcinogenic and Mutagenic
- Climate: Global Warming & Regional precipitation

# Dimethyl Ether (DME)



## Advantages

- **High oxygen content & the absence of C–C bonds**: smokeless combustion, low formation and high oxidation rates of particulates.
- **High cetane number**
- **Low boiling point**

## Disadvantages

- Low energy density
- High requirements on sealing materials

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# Sooting tendency

Quantitative sooting metrics were pronounced to evaluate sooting tendency among a wide range of hydrocarbon fuels, e.g., TSI, YSI.

## ❖ Threshold soot index (TSI) [1]

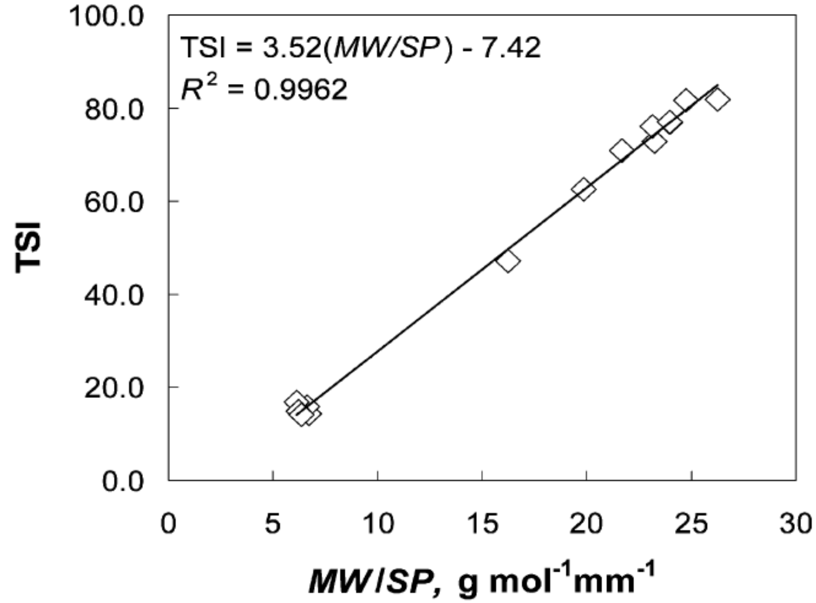


Fig. 3. Relationship between TSI and MW/SP ratio for prototype JP-900 fuel mixtures.

## ❖ Yield soot index (YSI) [2]

$$\mathrm{YSI} = C \times f_{\mathrm{v,max}} + D$$

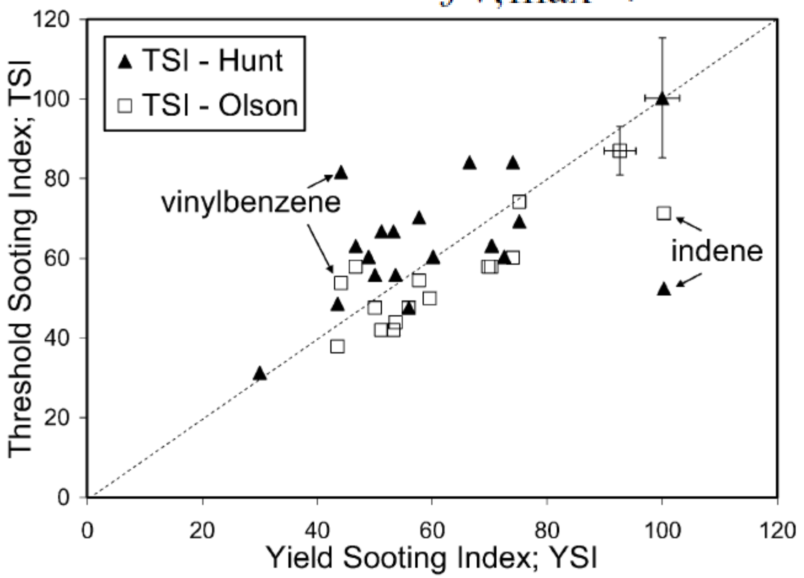


Fig. 6. Two sets of literature TSIs [9,27] plotted versus the measured YSIs. For clarity, error bars are shown for only one data point in each set; they represent the ±3% total uncertainty in YSI, the ±15% precision of TSI-Hunt, and the ±7% precision of TSI-Olson.

[1] Yang Y, Boehman AL, Santoro RJ. Combust Flame 2007;149:191–205.
[2] McEnally CS, Pfefferle LD. Combust Flame 2007;148:210–22.

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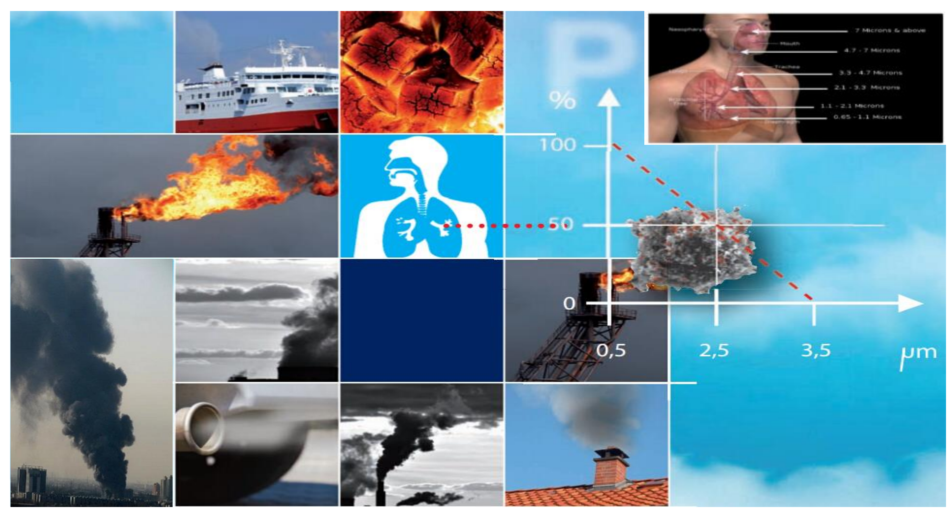
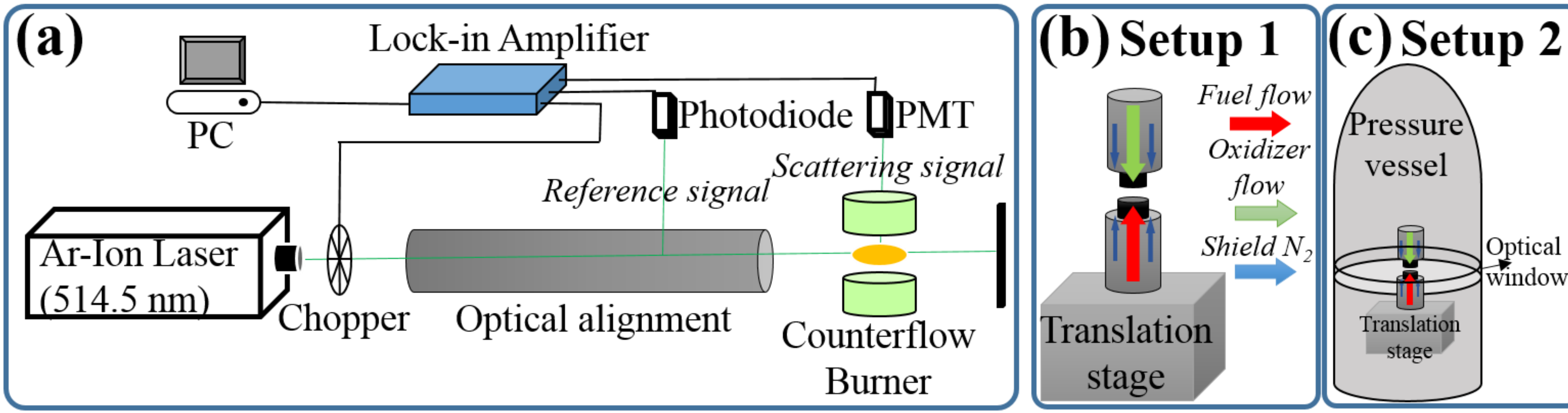


# Experimental setup

## Light scattering technique + Counterflow diffusion flames

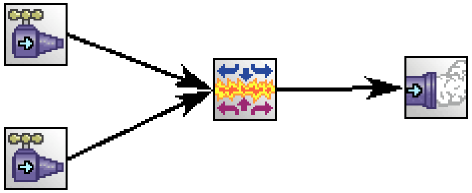



Schematics of experimental apparatus: Light scattering setup (a), and atmospheric counterflow burner (b)

# Numerical Simulation

**Flame temperatures and species concentrations** of experimental flames were computed using Chemkin Pro. A soot model is not included in the simulation due to the negligible impact of soot on flame temperature at the sooting limit.

- **Module**: Opposed-flow Flame package
- **Reaction kinetic model**: KAUST-Aramco PAH Mech 1 (KAM1)



[1] Park, Sungwoo, et al. "Compositional effects on PAH and soot formation in counterflow diffusion flames of gasoline surrogate fuels." *Combustion and Flame* 178 (2017): 46-60.

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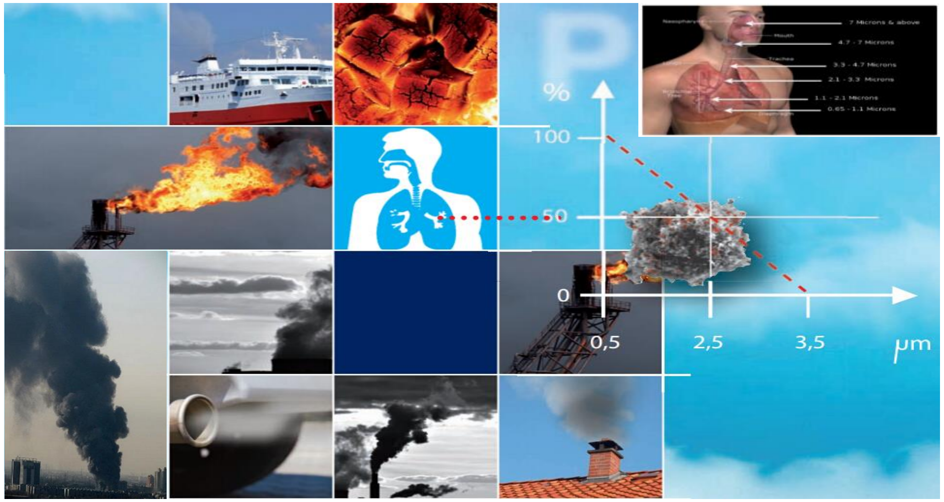


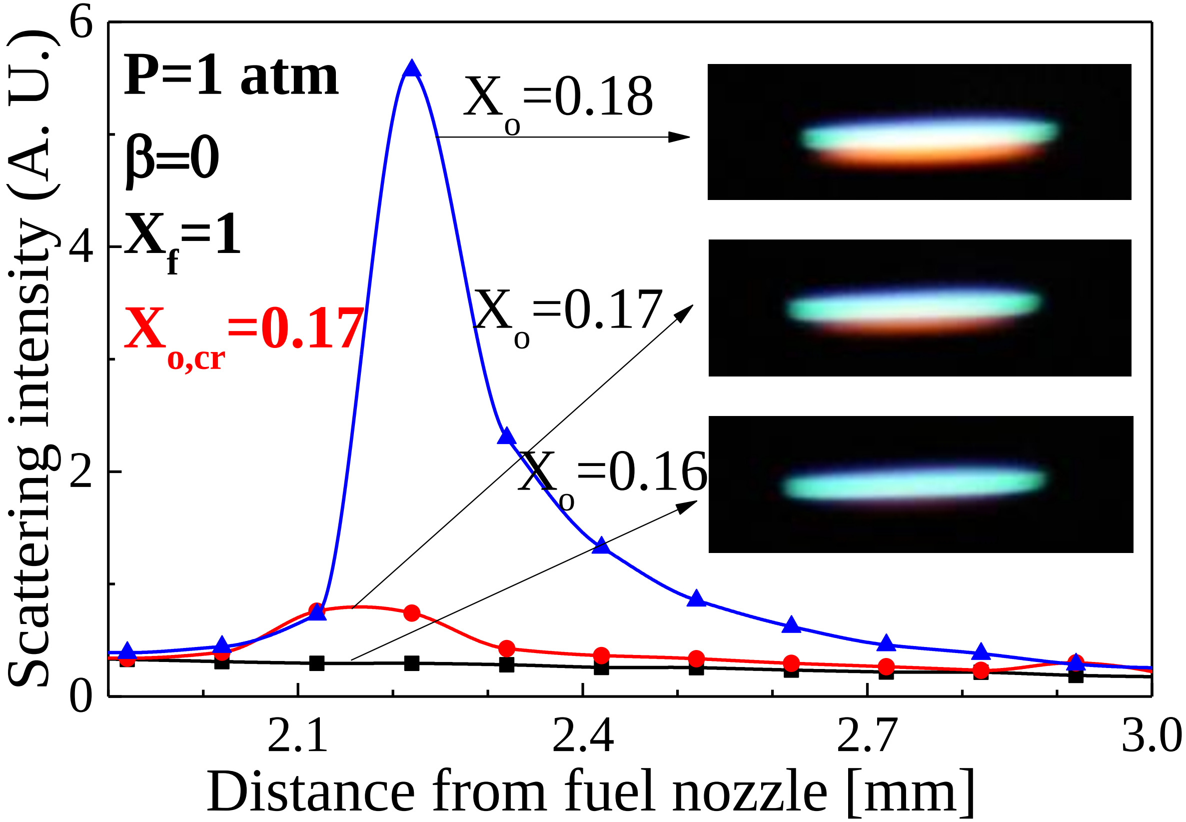
# How to determine sooting limits

The **sooting limit map** defined as the critical oxygen mole fraction ($X_o$) related to the fuel mole fraction ($X_f$) at soot inception point is detailed discussed in [1,2].

***Notation***

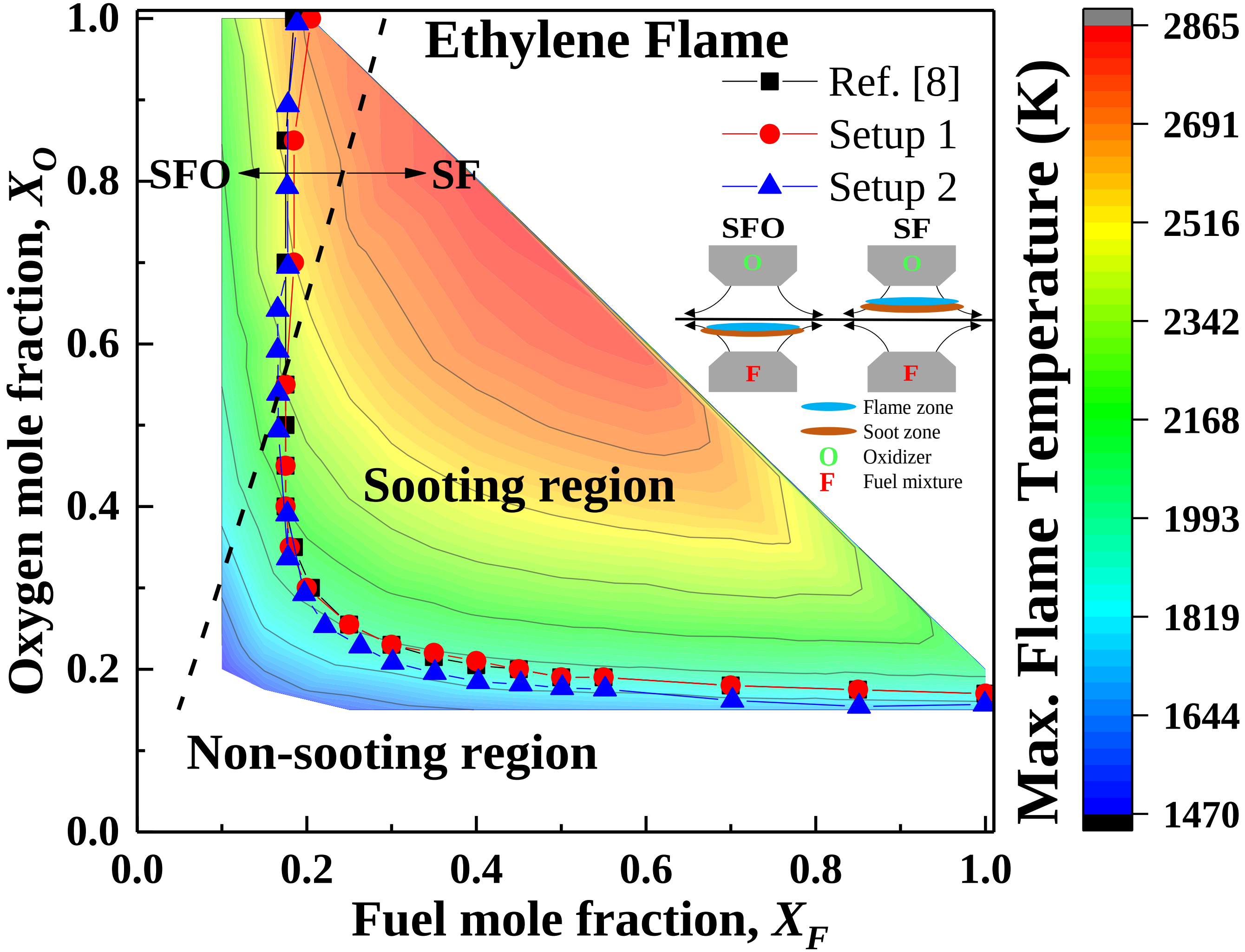
β: DME mixing ratio

$$\beta \equiv \frac{[C_2H_6O]}{[C_2H_6O]+[C_2H_4]}$$




[1] Y. Wang, S.H. Chung. Combust. Flame 161.5 (2014): 1224-1234.
[2] P.H. Joo, Y. Wang, A. Raj, S.H. Chung, Proc. Combust. Inst. 34 (2013) 1803–1809.

# Repeatability

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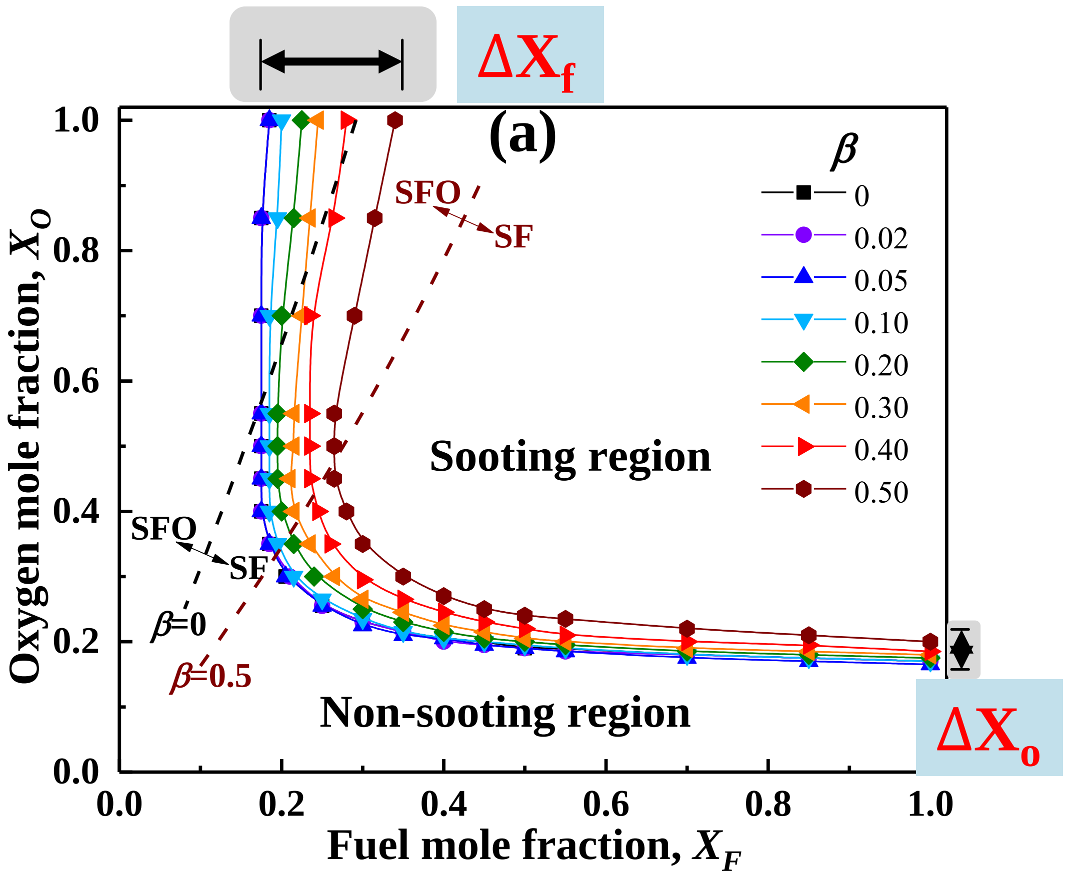
[2] P.H. Joo, Y. Wang, A. Raj, S.H. Chung, Proc. Combust. Inst. 34 (2013) 1803–1809.

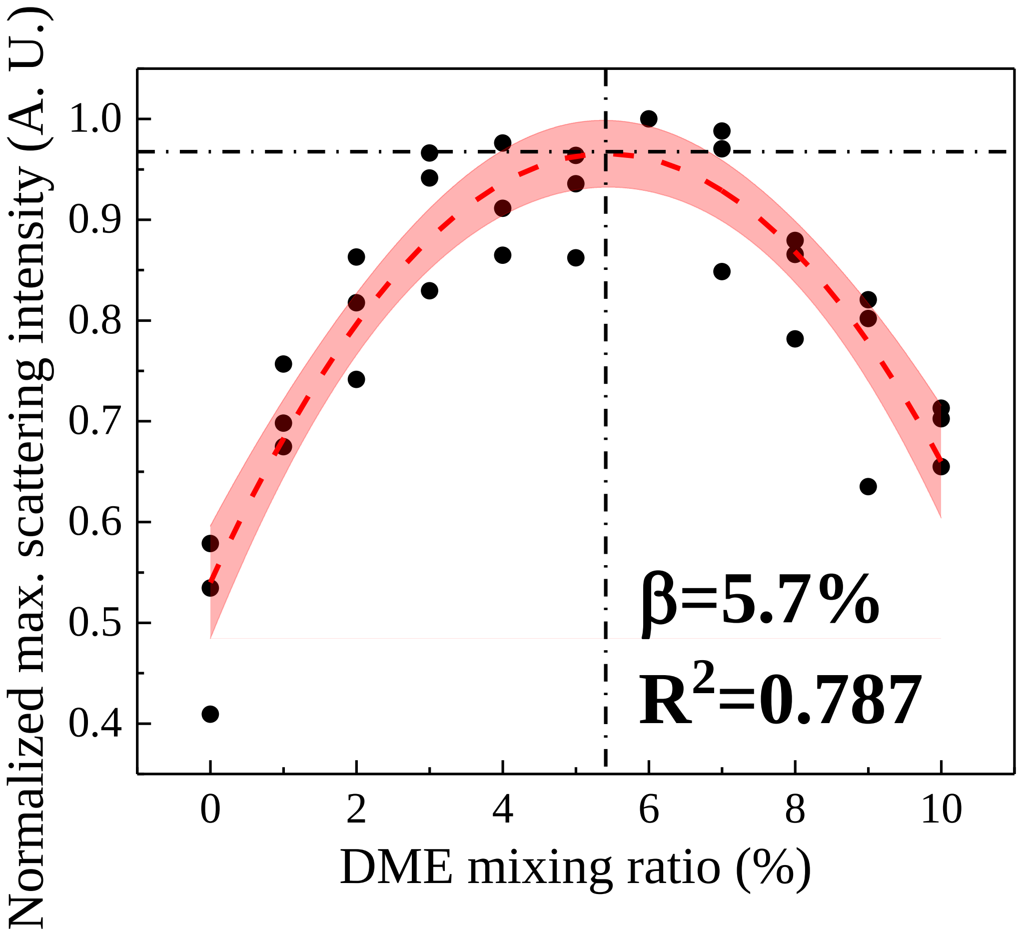
# 1. Sooting Limit Map




1. The addition of DME reduces sooting tendency among β=0.1-0.5.
2. $\Delta X_f > \Delta X_o$ : small thermal effect in SF flames, while high thermal effect in SFO flames.
3. Sooting limit curves are overlapped when β<0.1.

**Highest sooting propensity: 0~ 10% DME addition** ?

# 2. Highest sooting tendency

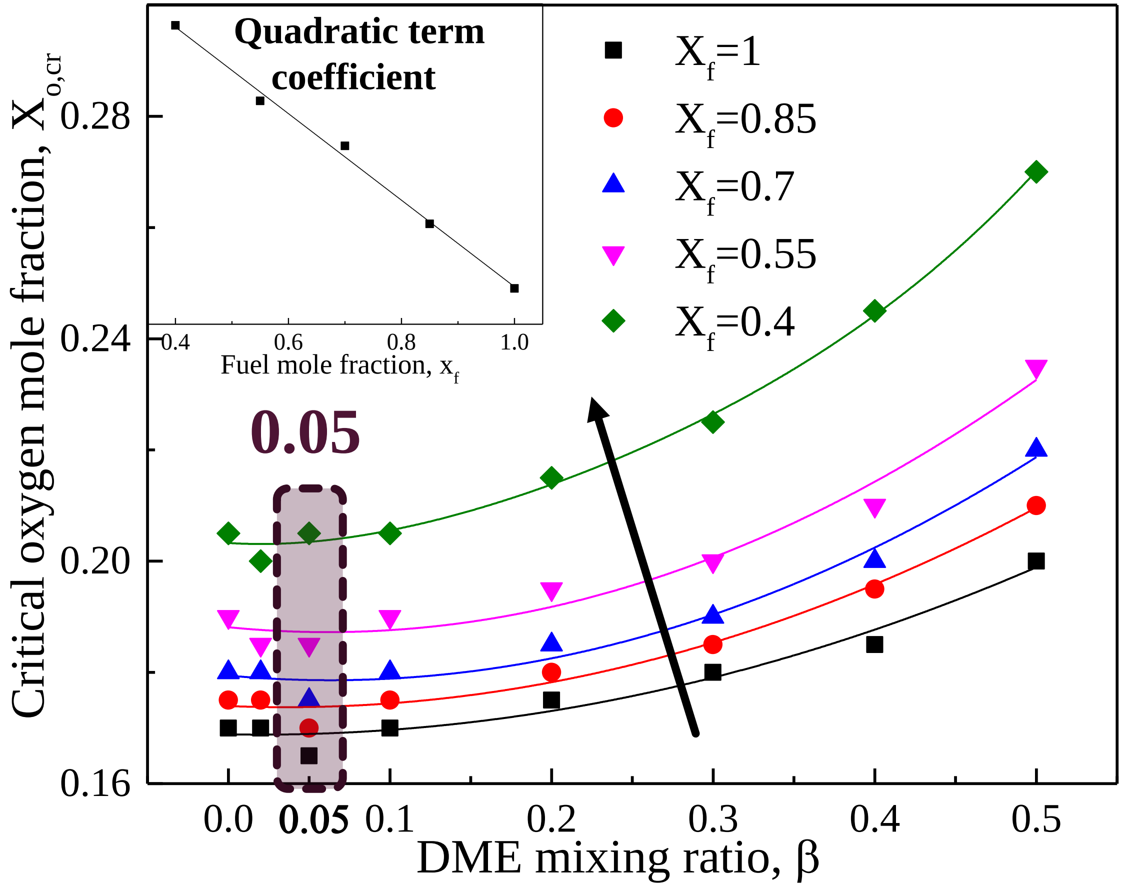



**Highest sooting propensity: *5.7%* DME addition**

**Critical DME mixing ratio = 5.7%**

Maximum scattering intensity as a function of DME mixing ratios (β) with 95% confidence band.

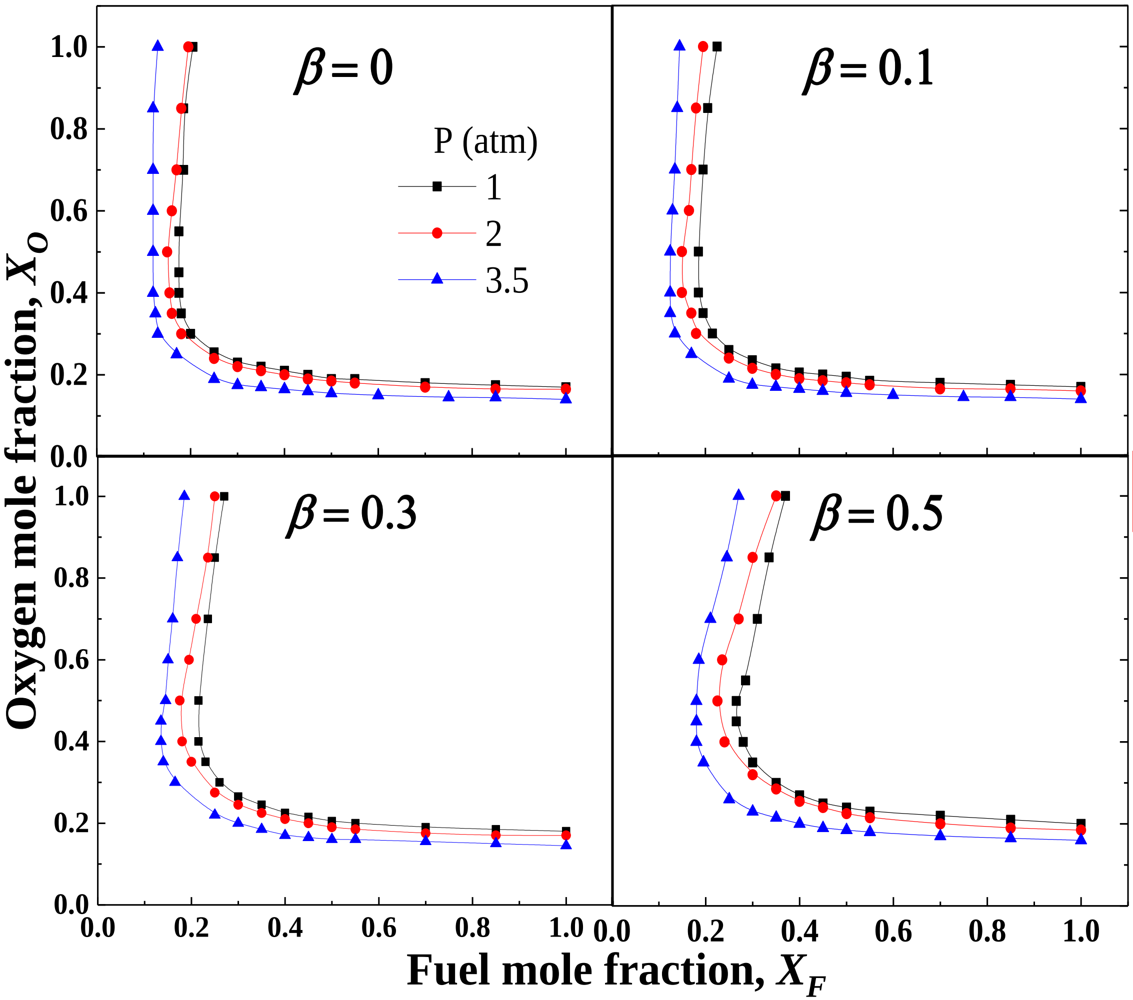
# 3. Dilution effect




Critical oxygen mole fraction as a function of DME mixing ratios (β)

**When the fuel (or carbon flow) is diluted, the dependence of dilution on sooting tendencies increases**

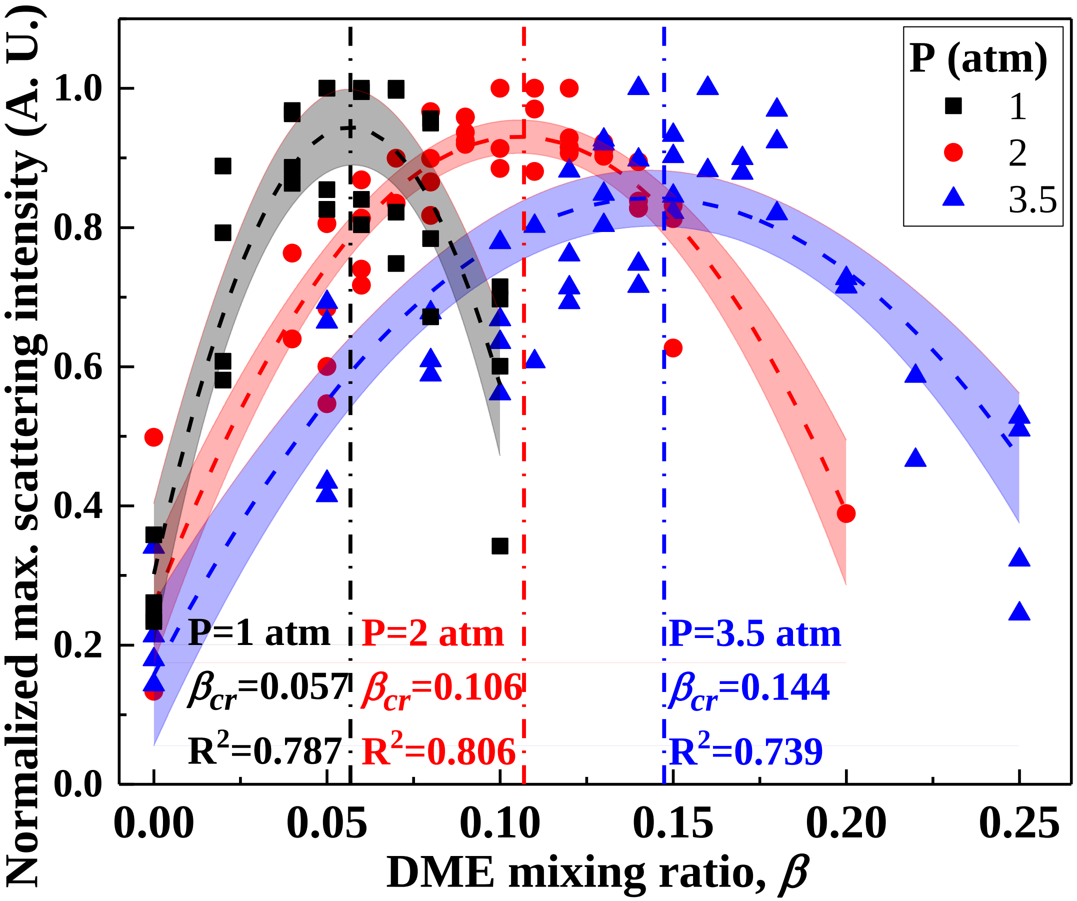
# 4. Pressure effect




**As pressure increases, sooting tendency increases**

Sooting limit maps with respect to DME mixing ratios ($\beta$) at P=1, 2, 3.5 atm

# 4. Pressure effect

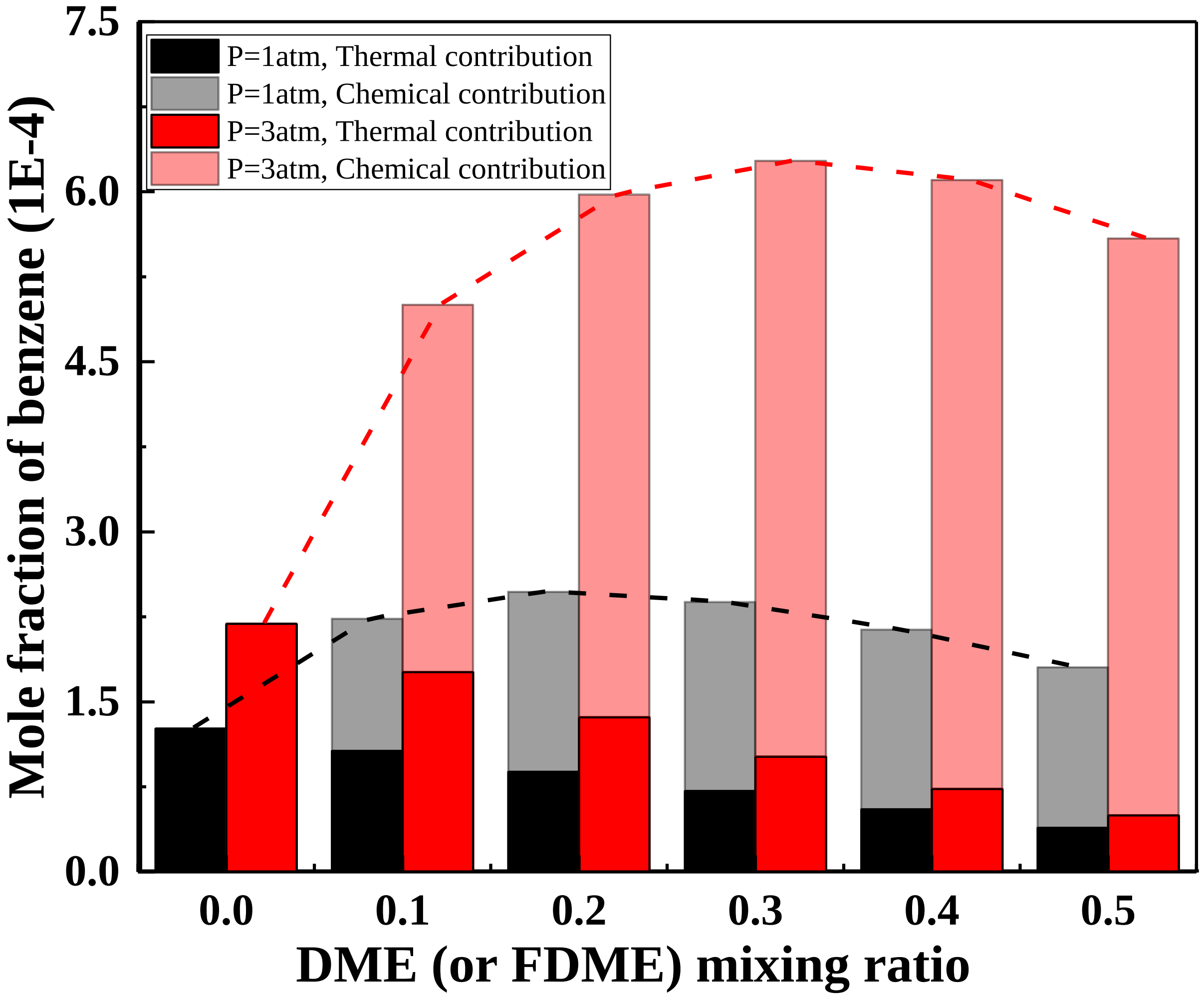



**The range of β in increasing soot propensity expands with pressure.**

**The effort to reduce soot by doping DME may not be effective at high pressures.**

Sooting propensity with DME mixing ratio at several pressures

# 5. Kinetic analysis




Thermal and chemical contributions to benzene production at $P$ = 1, 3 atm.

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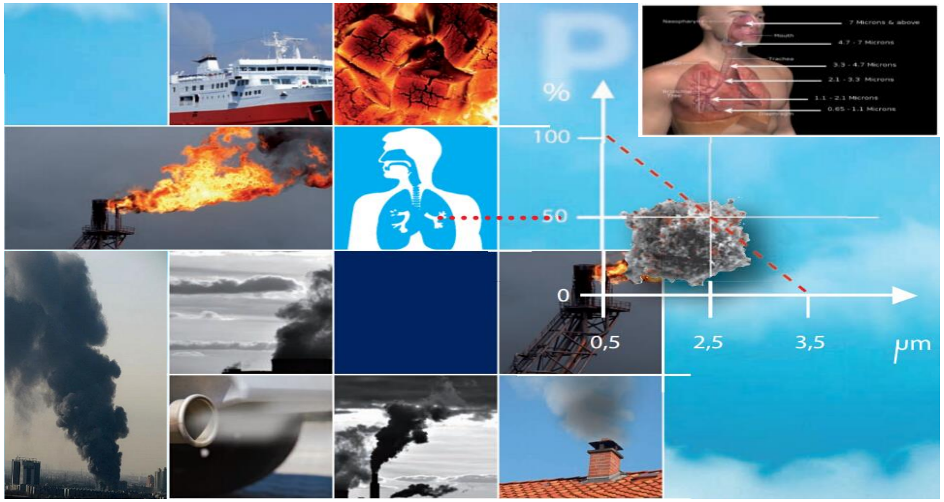

# Conclusions

- **The sooting limits ($X_f$ and $X_O$) are significantly sensitive to pressure, and the sooting tendency increases at higher pressure.** The range of β in increasing soot propensity with DME addition expands with pressure, thus the effort to reduce soot by doping DME may not be effective at high pressures.

- **When the fuel (or carbon flow) is diluted, the dependence of dilution on sooting tendencies increases.** That is, as $X_f$ decreases, the increase of $X_{o,cr}$ with respect to DME mixing ratio becomes more sensitive, meaning that the effect of DME addition on sooting tendency increases as the fuel is diluted.

- The behaviors of the DME effect on sooting limits in SF flame and SFO flame are slightly different. **Sooting tendency is more sensitive in SFO flames than in SF flames due to the thermal effect.**

- Kinetical analysis indicate **that soot formation with DME addition is dominantly determined by the synergistic chemical effect**, which is likely realized by the pathway of DME→$CH_3$(H)→$C_2H_2$($C_2H_3$&$C_3H_3$)→$C_6H_6$→soot.

# Acknowledgements

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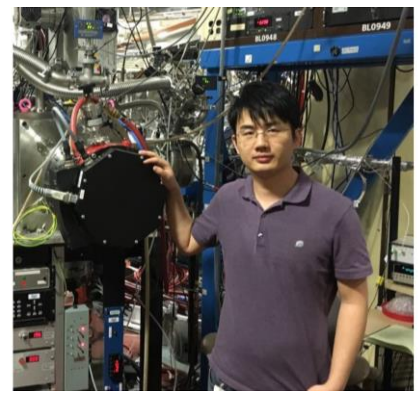
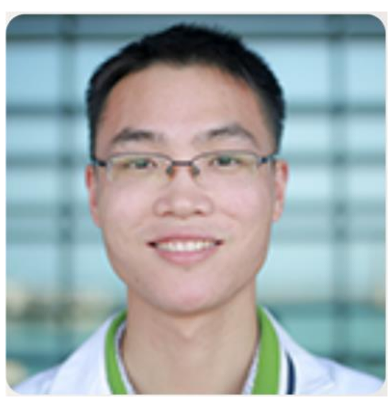


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