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Advancing the thermometric techniques at elevated pressure flames

Presented by

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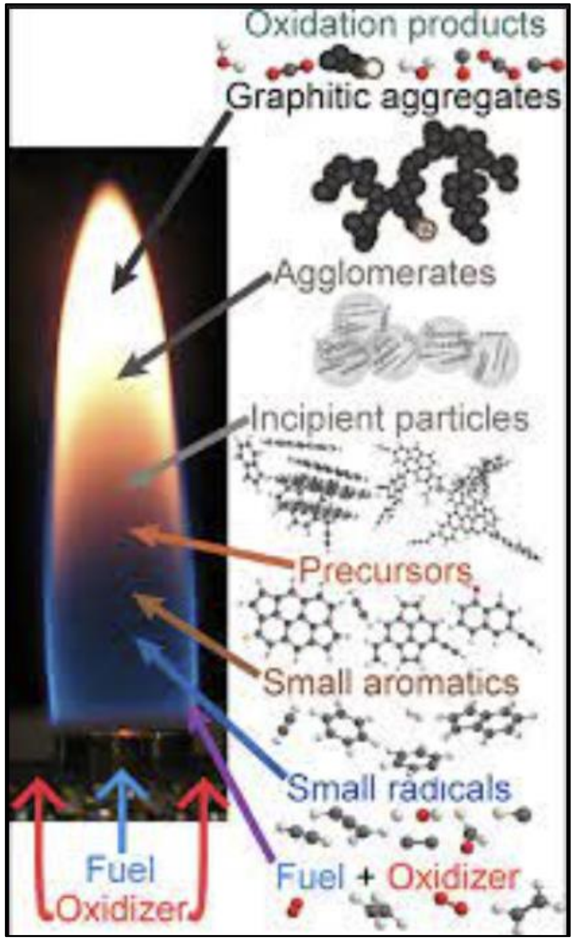
Outline

- Soot formation and evolution
- Role of temperature in soot formation and evolution
- Techniques: in practice and under development to achieve accuracy and precision
- Two Line Atomic Fluorescence (TLAF) : Theory
- Tracing elements: Temperature sensitivity & generation method
- TLAF work at atmospheric pressure conditions
- High pressure laser ablation system
- Planar temperature imaging under high pressure conditions
- Summary
- Future work
- References

Role of Temperature in soot formation and oxidation process



Basic chemistry process of soot formation and oxidation (Michelsen, 2017)

Monodisperse population balance model (MPBM)

MPBM predicts soot morphology by tracking the total agglomerate number, N, carbon molar, C, and surface area, A, concentrations.

$$\frac{dN}{dT} = -\frac{1}{2}\beta_m N^2 \qquad \beta_m = 4\sqrt{\frac{\pi k_B T}{m_{Ag}}}\; d_c^2$$

$\beta_m\, , collision\ frequency\ of\ the\ monodisperse\ agglomerates\ in\ the\ free\ molecular\ regime$

The rate of carbon addition by HACA surface growth

$$\left(\frac{dC}{dt}\right)^{Sg\ HACA} = 2\ \gamma\ \beta_{S,C_2H_2}\ [C_2H_2]\ N$$

Fraction of effective particle-molecule collisions,

$$\gamma = (\alpha K_s\, \chi_{soot} A_{Ag})/(\beta_{S,C2H2} N_{Av})$$

α is the fraction of actives sites

(Kholghy & Kelesidis, 2021)

Role of Temp in soot formation and oxidation process

Surface reaction rate constant for acetylene addition

$$K_s = 80 \cdot T^{1.56} \cdot e^{\left(\frac{-1912.4}{T}\right)}$$

$\beta_{S,C2H2}$ *is the collision frequency of the soot particles with acetylene molecules*

$$\beta_{S,C_2H_2} = \pi(d_g + d_{C_2H_2})^2 \sqrt{\frac{k_B T}{2\pi}\left(\frac{1}{m_{Ag}} + \frac{1}{m_{C_2H_2}}\right)}$$

The rate of carbon loss by O_2 oxidation

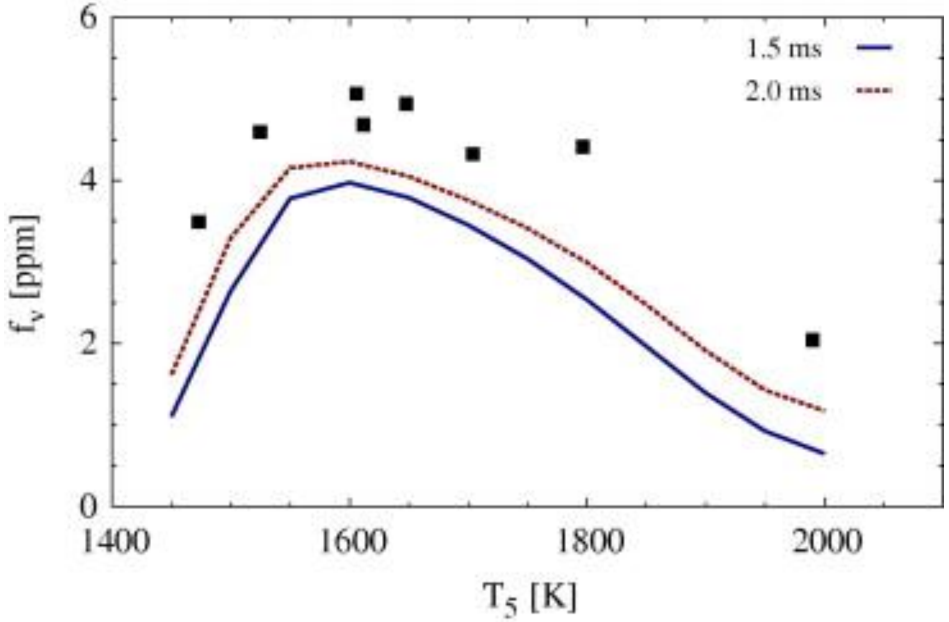
$$\left(\frac{dC}{dt}\right)^{Ox} = -\frac{\omega_{O_2} A}{MW_C}$$

The rate of change in A is related to dC/dt

$$\frac{dA}{dt} = \frac{4MW_C}{\rho\ d_p}\frac{dC}{dt}$$

Joint volume-surface-hydrogen model

Shock tube experiments

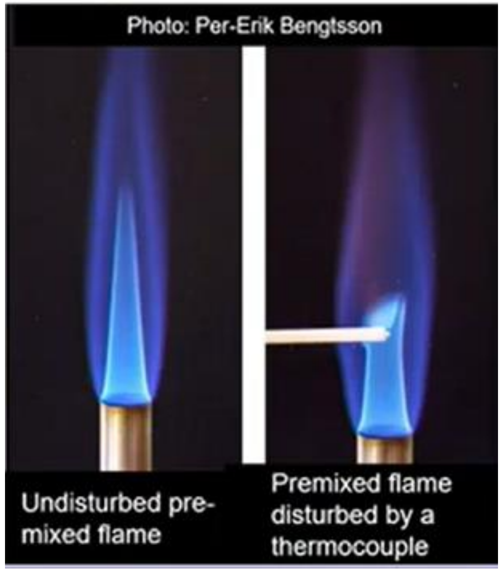


Evolution of the soot volume fraction with temperature (T5) for the pyrolysis of toluene in shock-tube. Symbols: experiments, solid line: predictions at 1.5 ms, dashed line: predictions at 2.0 ms. (Blanquart & Pitsch, 2009)

Temperature measurement techniques in gaseous flame

Intrusive measurements

- Thermocouple

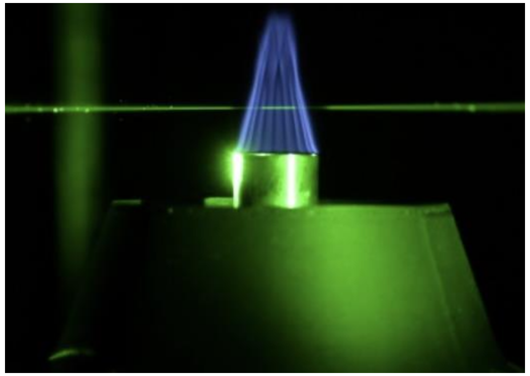


Source: https://youtu.be/m-ARPyGHkhE

Non-Intrusive measurements

Optical- diagnostics

- Laser induced fluorescence
- Rayleigh scattering measurement
- Filtered Rayleigh scattering measurements (FRS)
- Spontaneous Raman scattering (SRS)
- Rayleigh/Raman scattering measurements
- Coherent anti-Stokes Raman scattering (CARS)



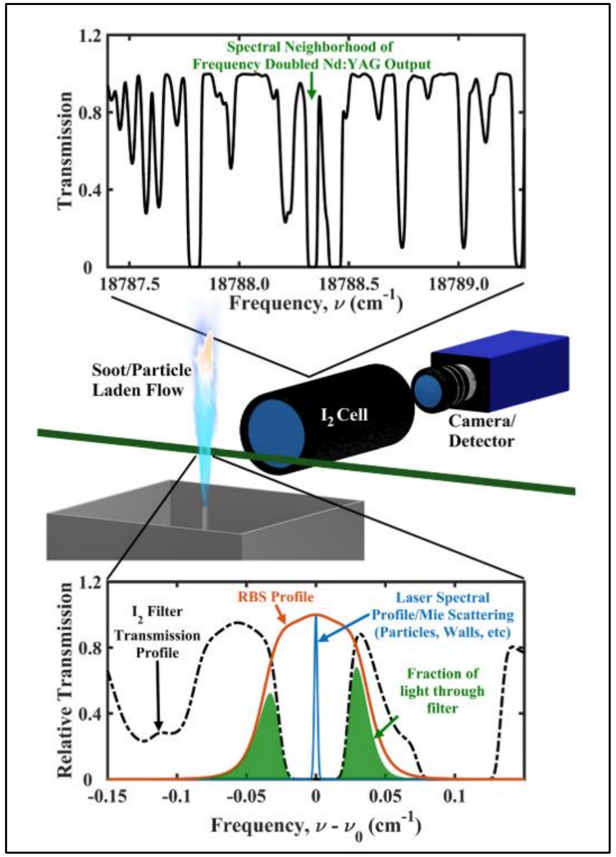
Source: https://www.rsm.tu darmstadt.de/index.en.jsp

Challenges in measuring temperature in particles laden flows

- **Background luminosity:** Increased background luminosity due to the soot particulate blackbody continuum radiation.
- **Laser-induced fluorescence:** Fluorescent interferences from soot precursors and particulates due to the abundance of such species in sooty flames.
- **Laser modulated particulate incandescence:** Increased quantities of the blackbody radiation and molecular emissions from the Cn species, when the soot particles absorb the incident laser radiation with sufficiently high flux
- **Absorption and scattering:** Extinction of the incident laser radiation through absorption and/or scattering when the carbonaceous particulates are present.

Techniques: in practice and under development to achieve accuracy and precision

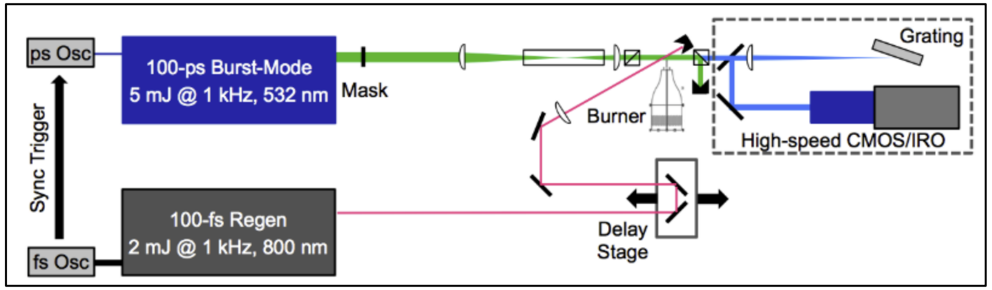
Filtered Rayleigh Scattering *(FRS)*



Graphical representation of the FRS working

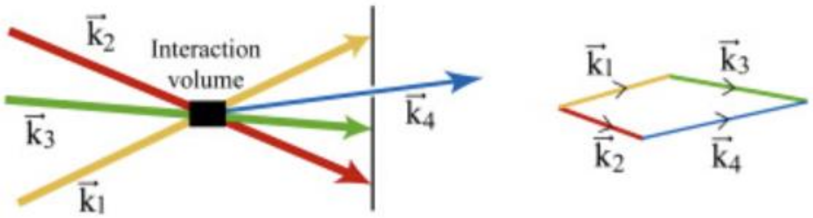
(McManus & Sutton, 2020)

Coherent Anti-Stokes Raman Scattering (CARS)



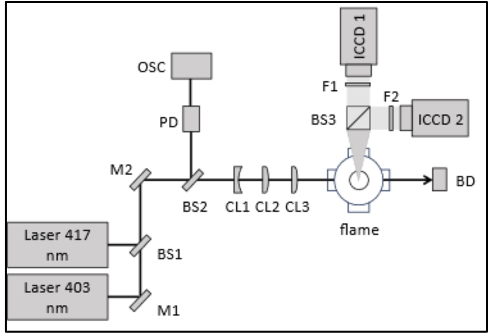
Experimental schematic showing optical layout and imaging system

(Iller et al., 2016)

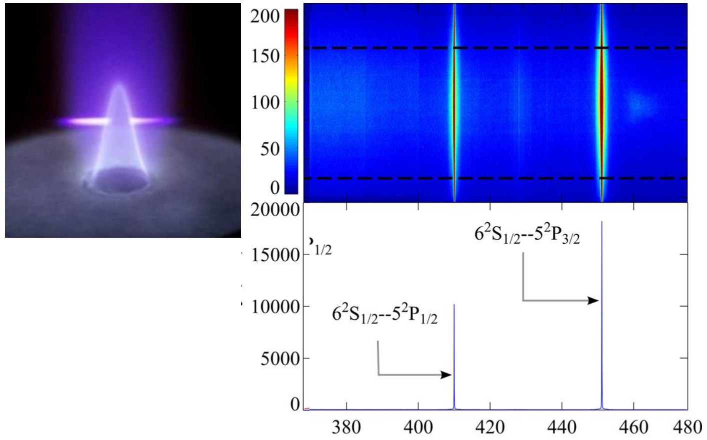


Vector diagram of laser beams

Two Line Atomic Fluorescence (TLAF)



Schematic of a TLAF setup



Fluorescence in flame and emission spectra at two line

(Whiddon et al., 2015)

Advantages and Limitations

Filtered Rayleigh Scattering (FRS)

Advantages

- Offer planar measurement
- One laser is required at fixed narrow line frequency
- Substantial suppression of background interferences

Limitations

- Low molecular scattering cross-section and sensitivity to surface and particles,
- Rayleigh scattering cross-section of each species in the mixture must be known
- Quantitative measurements requires simultaneous species information using SRS.
- Weak SRS signal make FRS challenging to perform in sooting /particle-laden flame

Advantages and Limitations

Coherent anti-Stokes Raman scattering (CARS)

Advantages

- Permit simultaneous detection of multiple species along with temperature
- Coherent, laser beam, like signal
- High signal to noise ratio
- Accuracy and precision are very high.

Limitations

- Complex and time-consuming optical alignment
- Challenging to do line and planar 2D-measurement
- Need to maintain perfect spatial overlap between multiple lasers beams, minor misalignment can result signal loss.
- Limited implementation in harsh environment due to challenge in maintaining spatial overlap under high pressure, temperature gradient, turbulent flame

Advantages and Limitations

Two Line Atomic Fluorescence (TLAF)

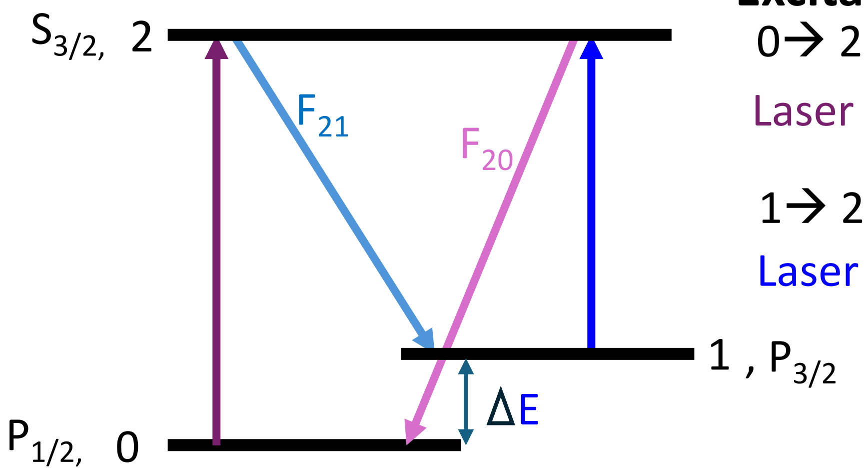
Advantages

- Off resonance measurement
- Offer planar measurement
- Independent of gas composition
- Ratio of fluorescence is independent of quenching
- Accuracy is similar to CARS

Limitations

- Oxidation of tracer particles in the vicinity of reaction zone
- Interference due to broadband nature of LII signal in sooting flame

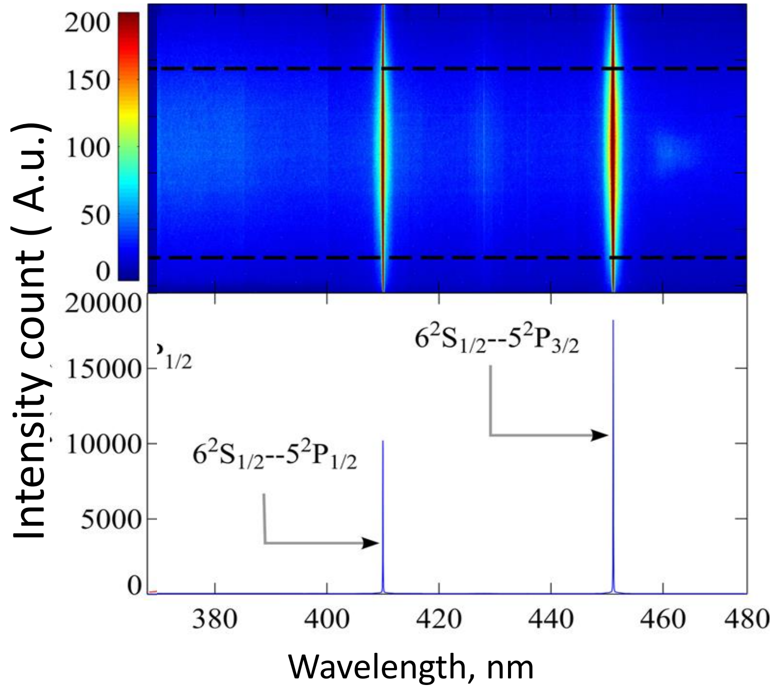
Two Line Atomic Fluorescence (TLAF): Background



Excitation		**Fluorescence**
0→ 2 Laser 403nm	→	2→ 1 LIF 417 nm
1→ 2 Laser 417 nm	→	2→ 0 LIF 403 nm

Electronic configuration of a 3-level lambda system commonly used in TLAF

(Alkemade C.,1970)
(Omenetto et al., 1972)
(Aldén et al., 1983)
(Borggren et al., 2017)

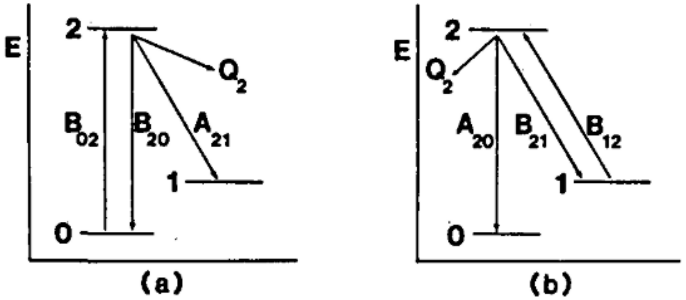


Indium emissions spectra of the two lines
(Whiddon et al., 2015)

Benefits :

- Seeding makes it independent of the gas composition
- Atomic fluorescence stronger than molecular fluorescence
- Off resonance, hence insensitivity to elastic scattering
- Ratio of LIF signal mitigate the dependence on Quenching rate

Two Line Atomic Fluorescence (TLAF): Theory



Two line fluorescence process

(Joklik & Daily, 1982)

$$n_2 = \frac{n_1 W_{12}}{W_{21} + A_{21} + A_{20} + Q_2}$$

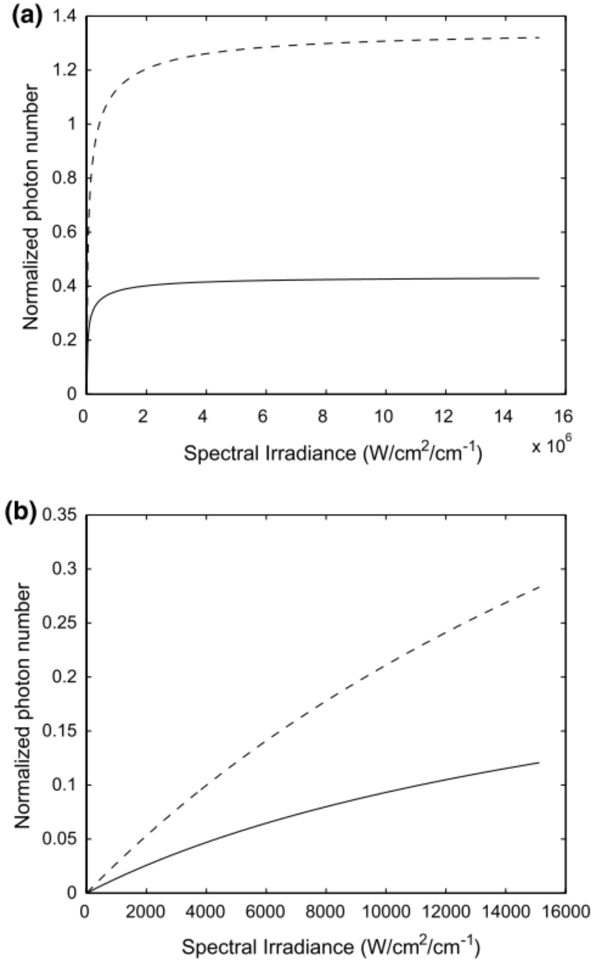
$$W_{12} = B_{12} I_{12}$$

$$n_2 = \frac{n_0 W_{02}}{W_{20} + A_{21} + A_{20} + Q_2}$$

$$W_{02} = B_{02} I_{02}$$

$$F_{i\rightarrow 2} = h\nu_{2i}\, n_2 A_{2i} \frac{\Omega}{4\pi}$$

$$\frac{n_1}{n_0} = \frac{g_1}{g_0} exp\left(\frac{-\Delta E_{10}}{kT}\right)$$



a) Fluorescence Vs pulse energy

b) Zoomed in view of approx. linear regime

(Manteghi et al., 2015)

Linear regime (Borggren et al., 2017)

$$W_{21} \ll A_{21} + A_{20} + Q_2$$

$$T = \frac{\Delta E_{10}/k}{4ln\left(\frac{\lambda_{21}}{\lambda_{20}}\right) + ln\left(\frac{F_{20}}{F_{21}}\right) - ln\left(\frac{I_{12}}{I_{02}}\right) + ln\, C_T}$$

Saturation regime (Medwell et al., 2009)

$$W_{21} \gg A_{21} + A_{20} + Q_2$$

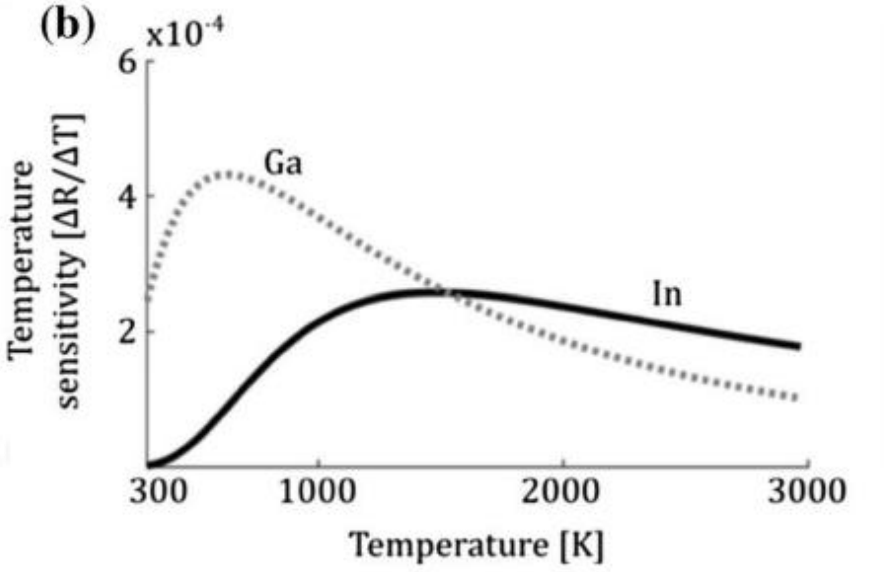
$$T = \frac{\Delta E_{10}/k}{ln\left(F_{21} * (1 + \frac{C_s}{I_{20}}\right) - ln\left(F_{20} * (1 + \frac{C_{As}}{I_{21}}\right) + C_T}$$

$$C_s = 1 + \frac{Q + A}{B_{20}} \qquad C_{As} = 1 + \frac{Q + A}{B_{21}}$$

Tracing element: temperature sensitivity & seeding method

Temperature sensitivity two metal atoms

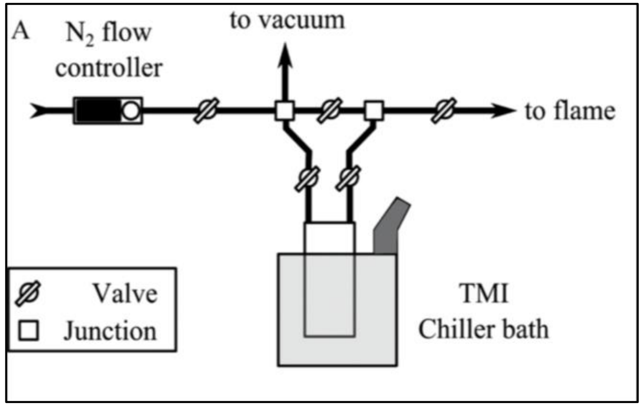
$$R_{\mathrm{sim}}(T) = \frac{g_{12}\left(\lambda_{12}, T\right) \cdot f_1(T) \cdot B_{12}}{g_{02}\left(\lambda_{02}, T\right) \cdot f_0(T) \cdot B_{02}},$$



Simulated temperature sensitivity of Ga and In

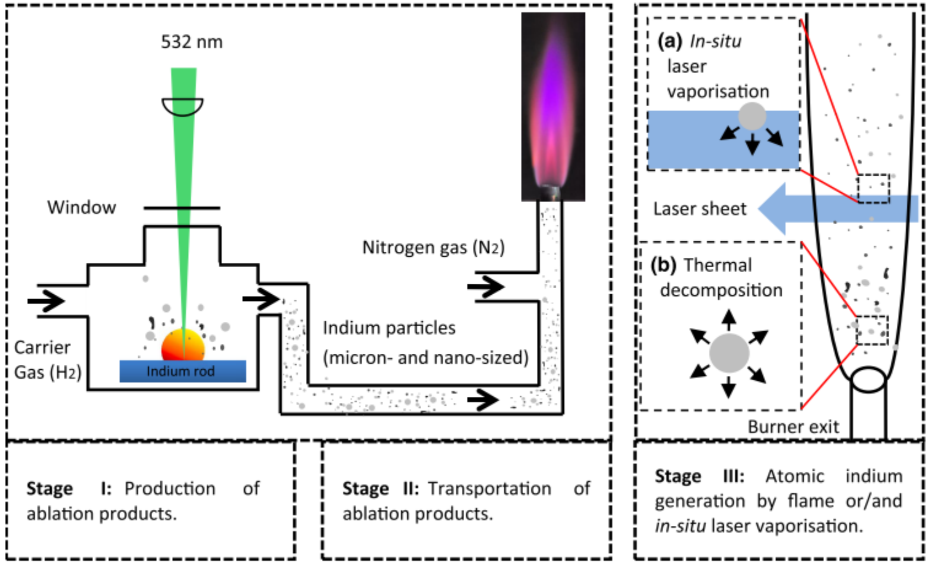
(Borggren et al., 2017)

Seeding method



Tri-methyl-Indium seeding set up

(Whiddon et al., 2015)



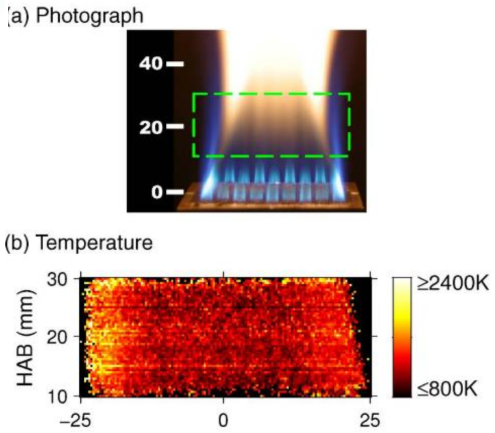
Stage I: Production of ablation products.

Stage II: Transportation of ablation products.

Stage III: Atomic indium generation by flame or/and *in-situ* laser vaporisation.

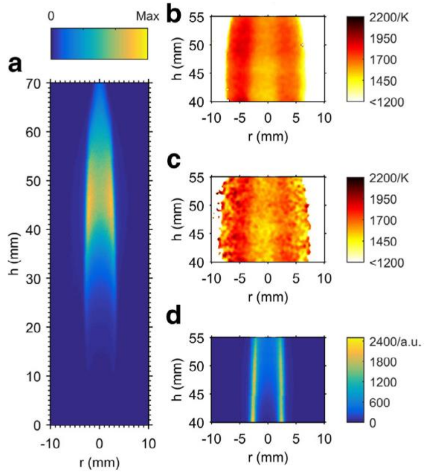
Ablation process (Gu et al., 2015)

TLAF work at atmospheric conditions



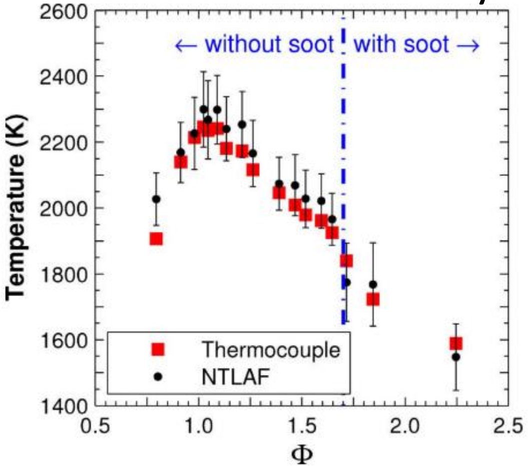
a) Ethylene/air flame, Phi 2.25,
b) b) Inst. NTLAF temp.

Ethylene/air flame, Phi 2.25



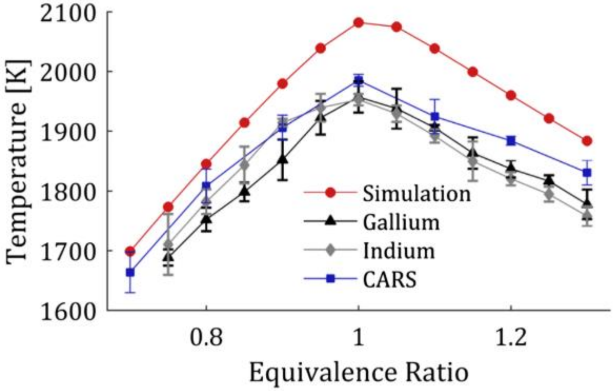
a) Flame Luminosity b) Tavg c) Inst. Temp.

Accuracy ≤ 30 K



Temperature of flame over range of Phi for NTLAF and calibrated thermocouple (Medwell et al., 2009)

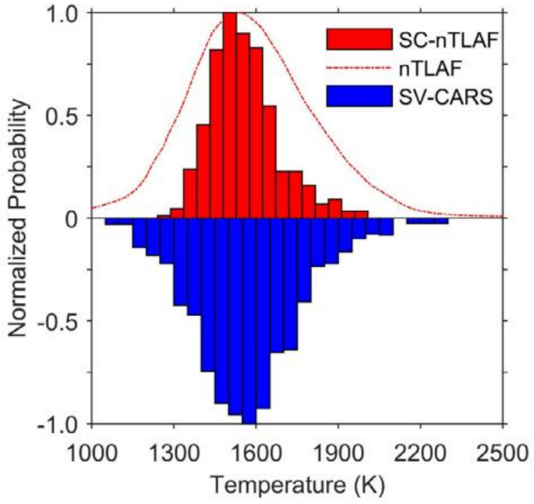
Precision ~1.1 %
Accuracy~ 2.7%



Temperature measured in multi-jet burner

(Borggren et al., 2017)

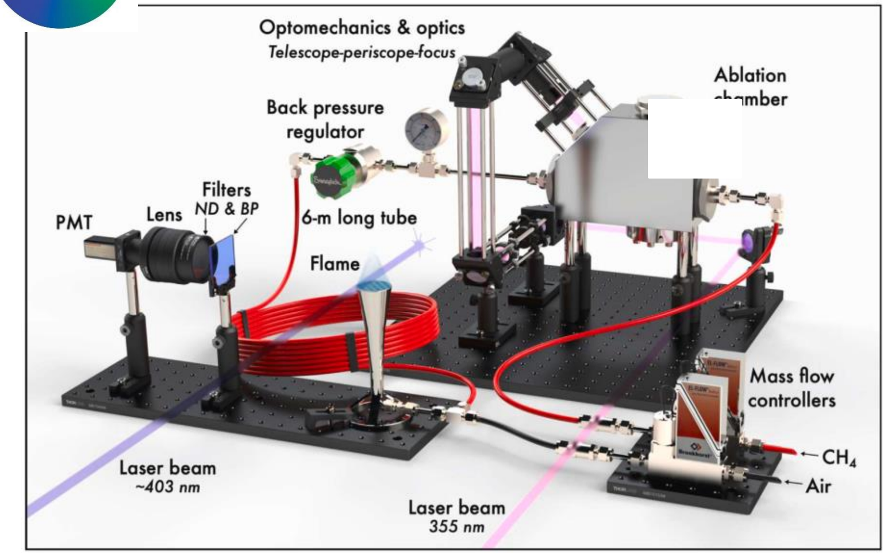
σ_T/T_{mean}~4.1 % or ±70K

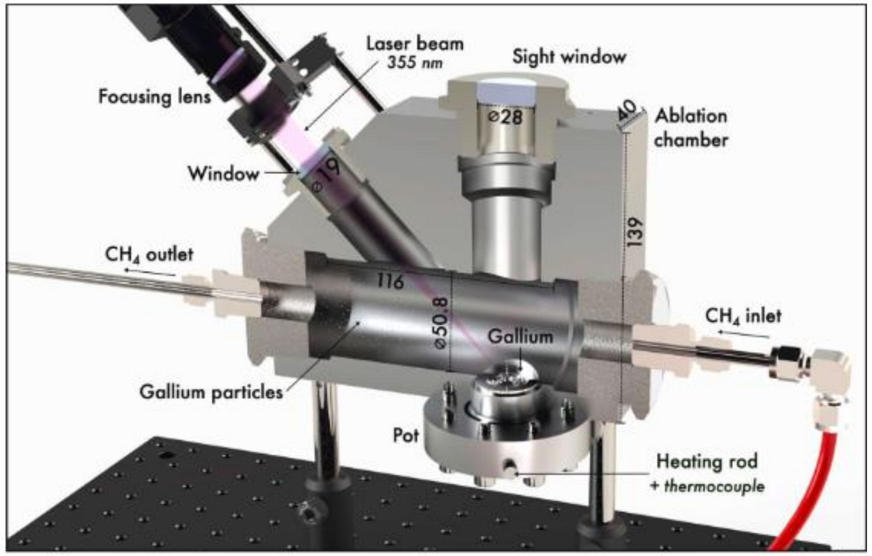


Histogram of Temperature

(Sun et al., 2019)

High pressure laser ablation system



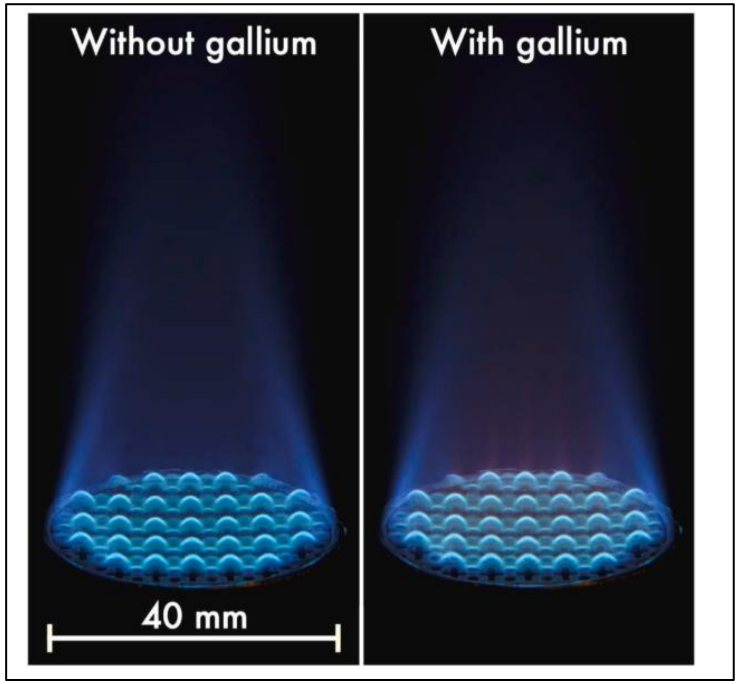


Desing to fulfill the following requirement

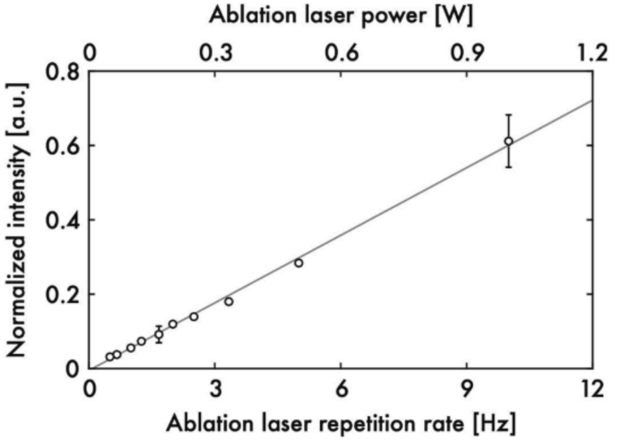
- Operating pressure up to 30bar
- Feature a pot filled with gallium feedstock
- Optical window to allow laser beam enter inside
- Provision to heat the gallium feedstock to its liquid phase
- Avoid any foreign metal subject to forming a structurally weak amalgam in contact with gallium.
- Laser ablation seeding unit cable of introducing gallium particles into a gaseous flow an elevated pressures

(Guiberti et al., 2024)

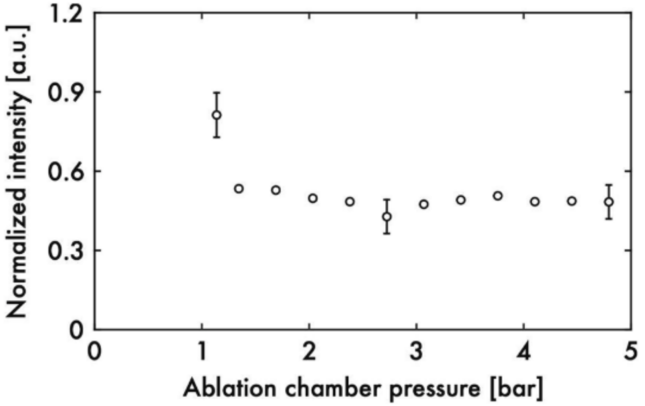
High pressure laser ablation system: continue



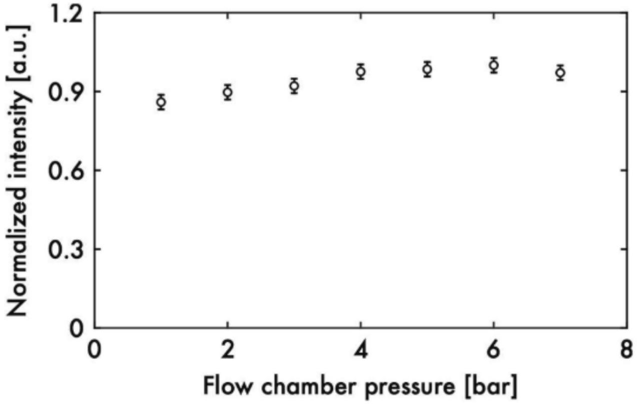
Time averaged broadband flame image Recorded with a DSLR camera in CH4



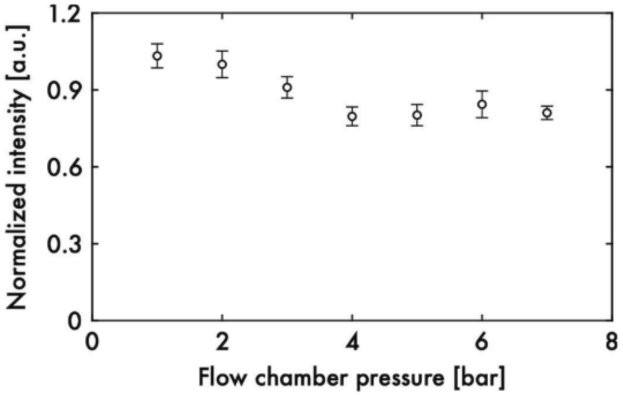
LIF intensity in flame Vs ablation laser repletion rate.



LIF intensity Vs the ablation chamber's pressure.



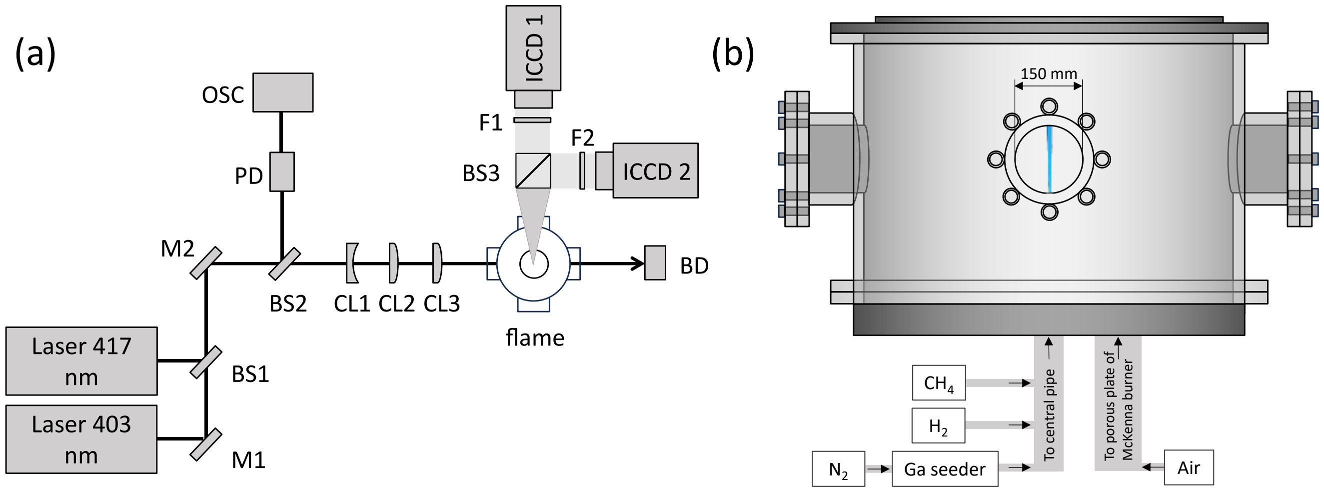
Laser scattering Vs flow chamber's pressure.



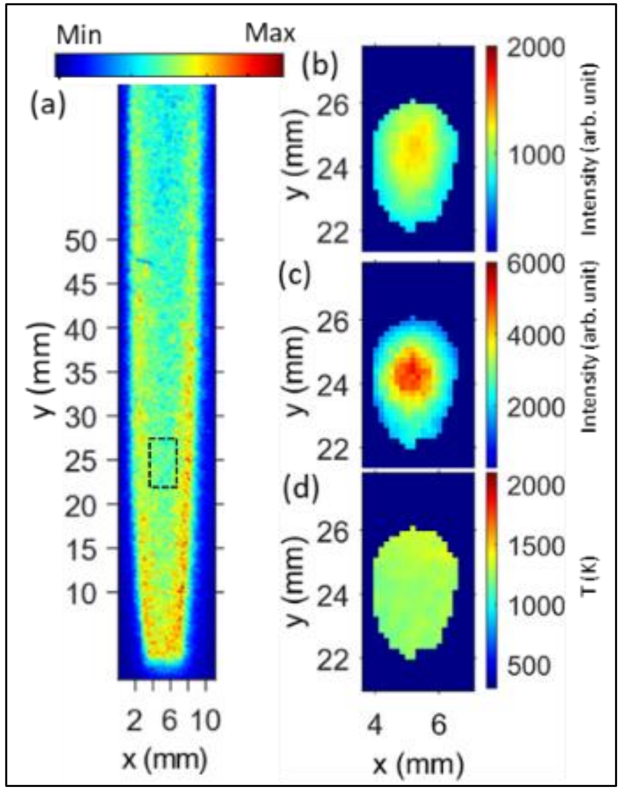
LIF intensity Vs flow chamber's pressure.

Planar temperature imaging under high pressure conditions

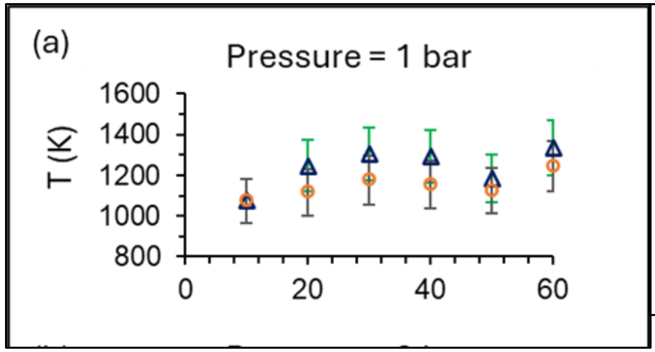
Experimental setup



LIF signal at 6 bars in laminar flame



(a) Chemiluminescence image of laminar H2-CH4 air diffusion jet flame captured at 403nm; Typical examples of TLAF images of the laminar flame jet core at 6 bars and HAB = 20 mm,



- An agreement of ±**130 K**, between Rayleigh scattering and TLAF Temperature
- Uncertainty in TLAF measurement ~ ±**15 %**

5H02: ***Temperature imaging of elevated pressure flames using planar laser induced fluorescence***

Planar temperature imaging under high pressure conditions: continue

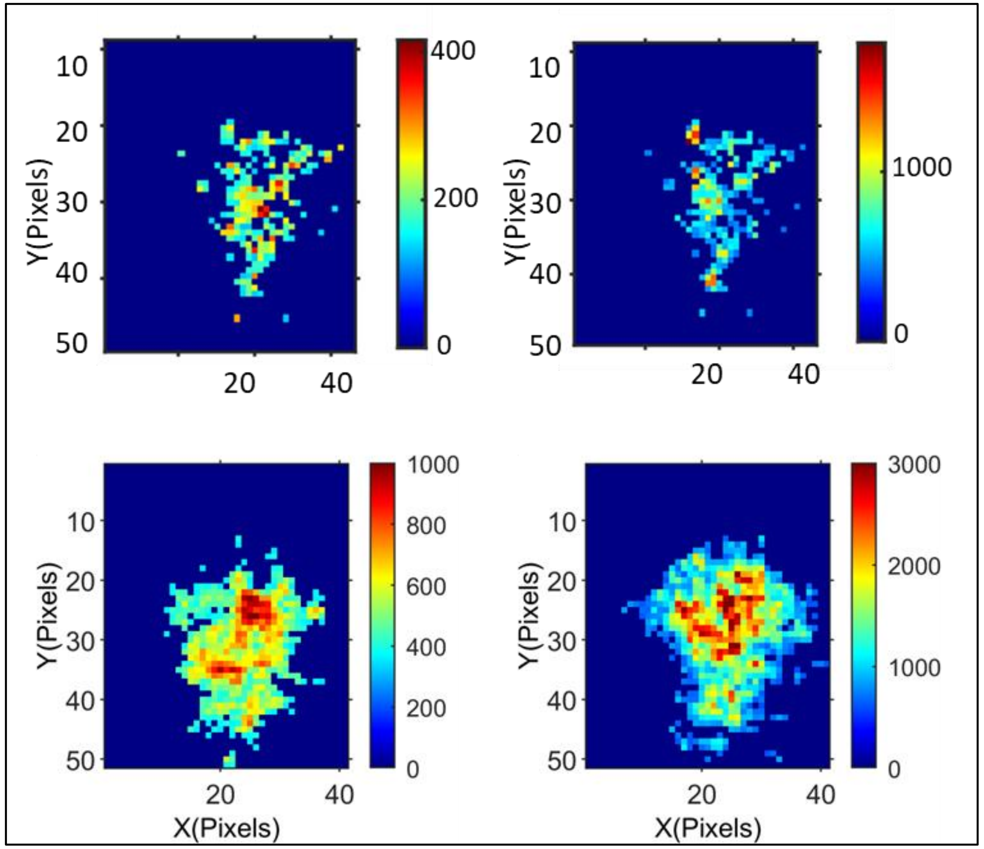
LIF signal in turbulent flame

Re ~ 4000

Filter LIF 403nm Filter LIF 417nm

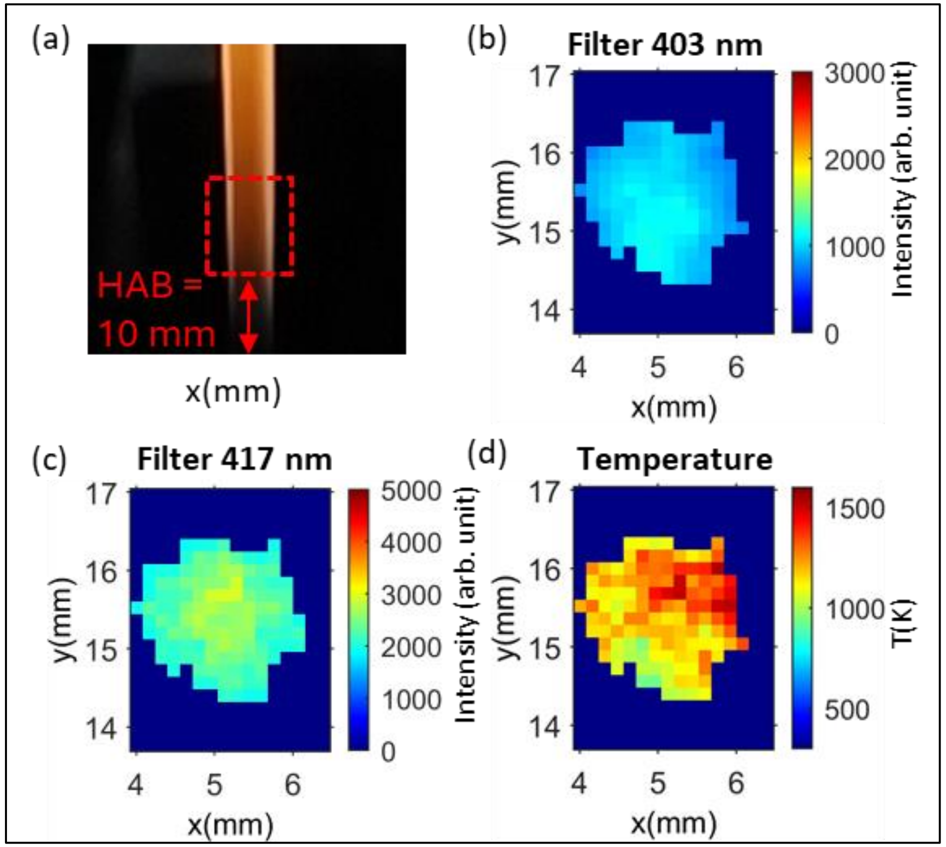
1 bar

5 bar



Laminar sooting flame at 5 bar

Re ~ 2300



5H02: ***Temperature imaging of elevated pressure flames using planar laser induced fluorescence***

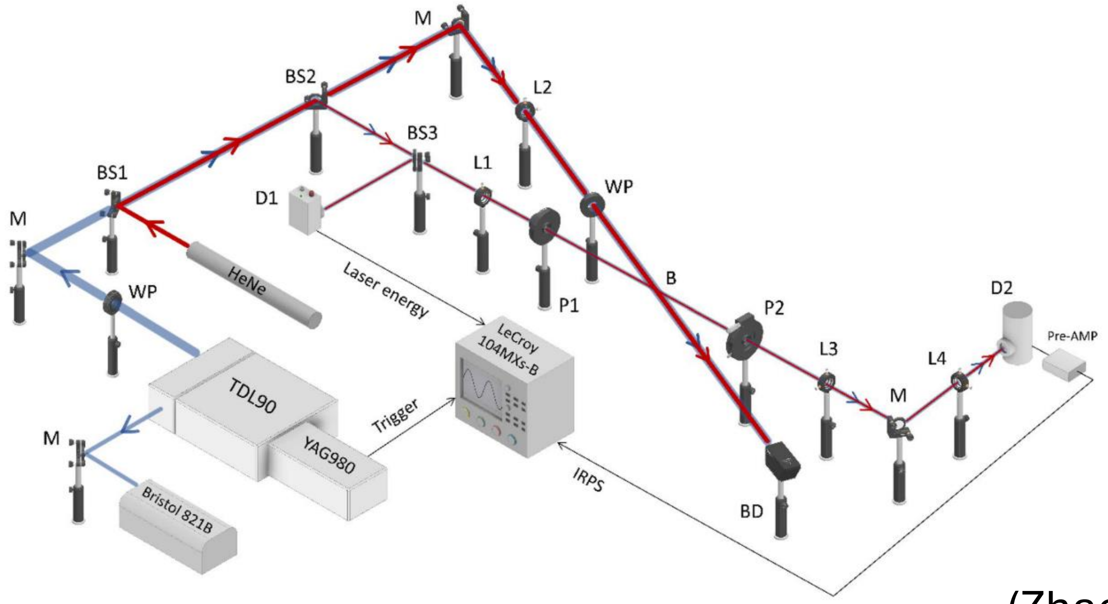
Summary

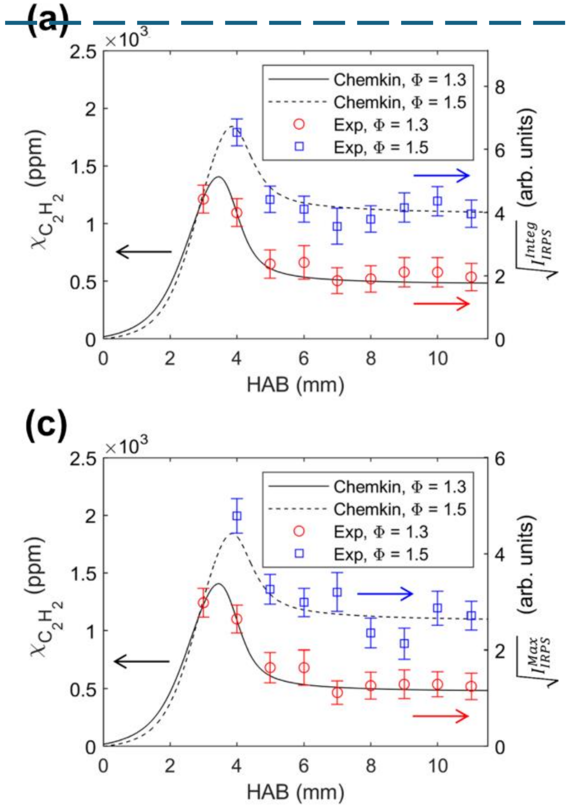
- Soot formation process scales non-linearly with temperature .
- Accurate temperature information is necessary to improve the understanding of soot formation and evolutions in order to improve the existing model
- TLAF hold promise for more precise and accurate planar imaging of temperature in particle laden flow specially in sooty environment .
- TLAF work at atmospheric pressure shows acceptable accuracy and precision in temperature values.
- The newly designed high pressure ablation chamber works well to seed the flame at high pressure.
- TLAF temperature data shows the potential of techniques to measure temperature under high pressure conditions.

Future work

- Improving the seeding concentration and signal-to noise ratio in flame
- Implementation of non-linear TLAF regime at elevated pressure conditions
- Use of ultra-narrow bandpass filter to suppress the LII broadband signal in sooting flame at high pressure.

- **C2H2 measurements using mid-infrared polarisation spectroscopy**





(Zhao et al., 2023)

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