Propagation of laminar flames of light and heavy fuels at engine-relevant conditions: state-of-the-art and future direction

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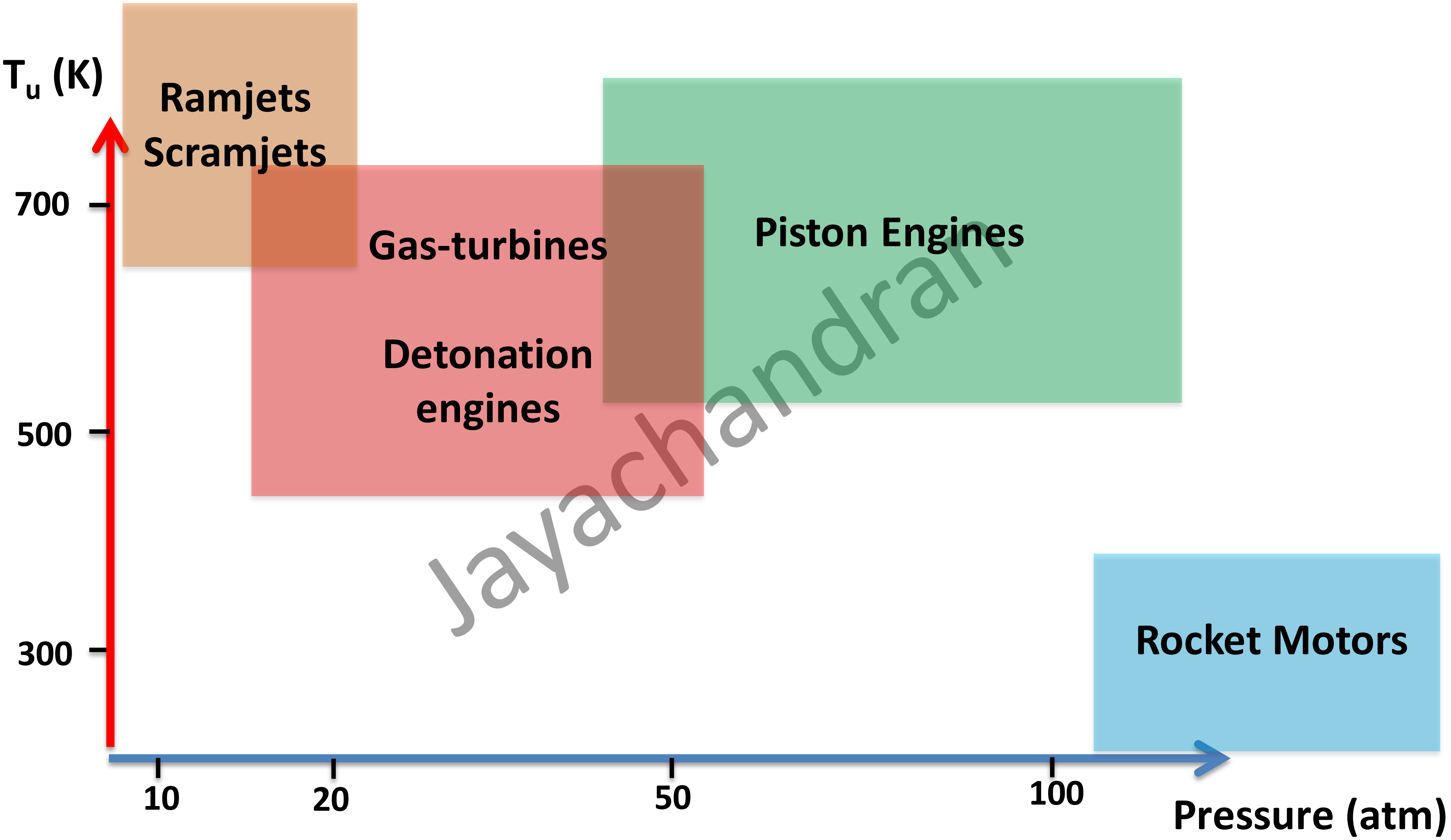
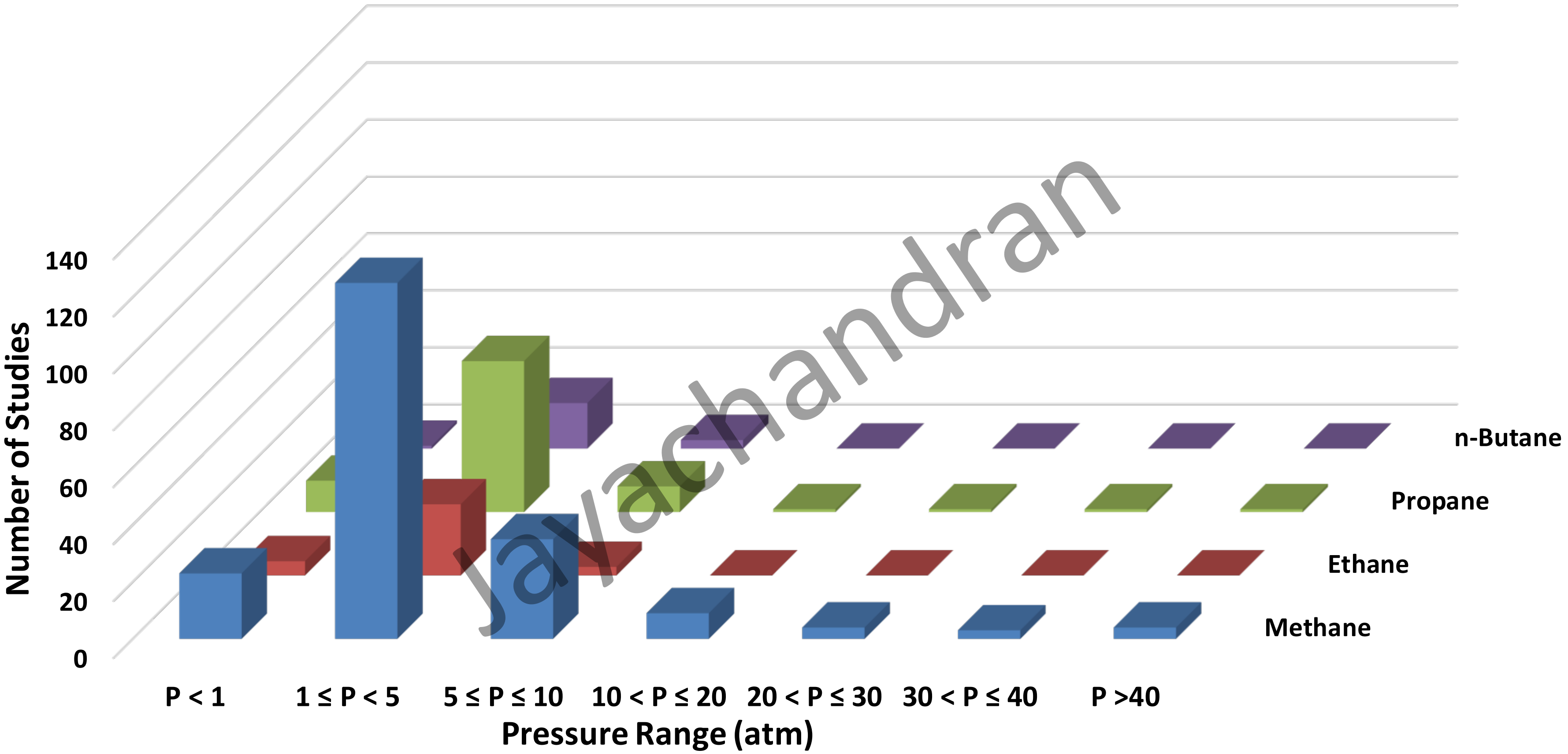
Engine-relevant thermodynamic conditions

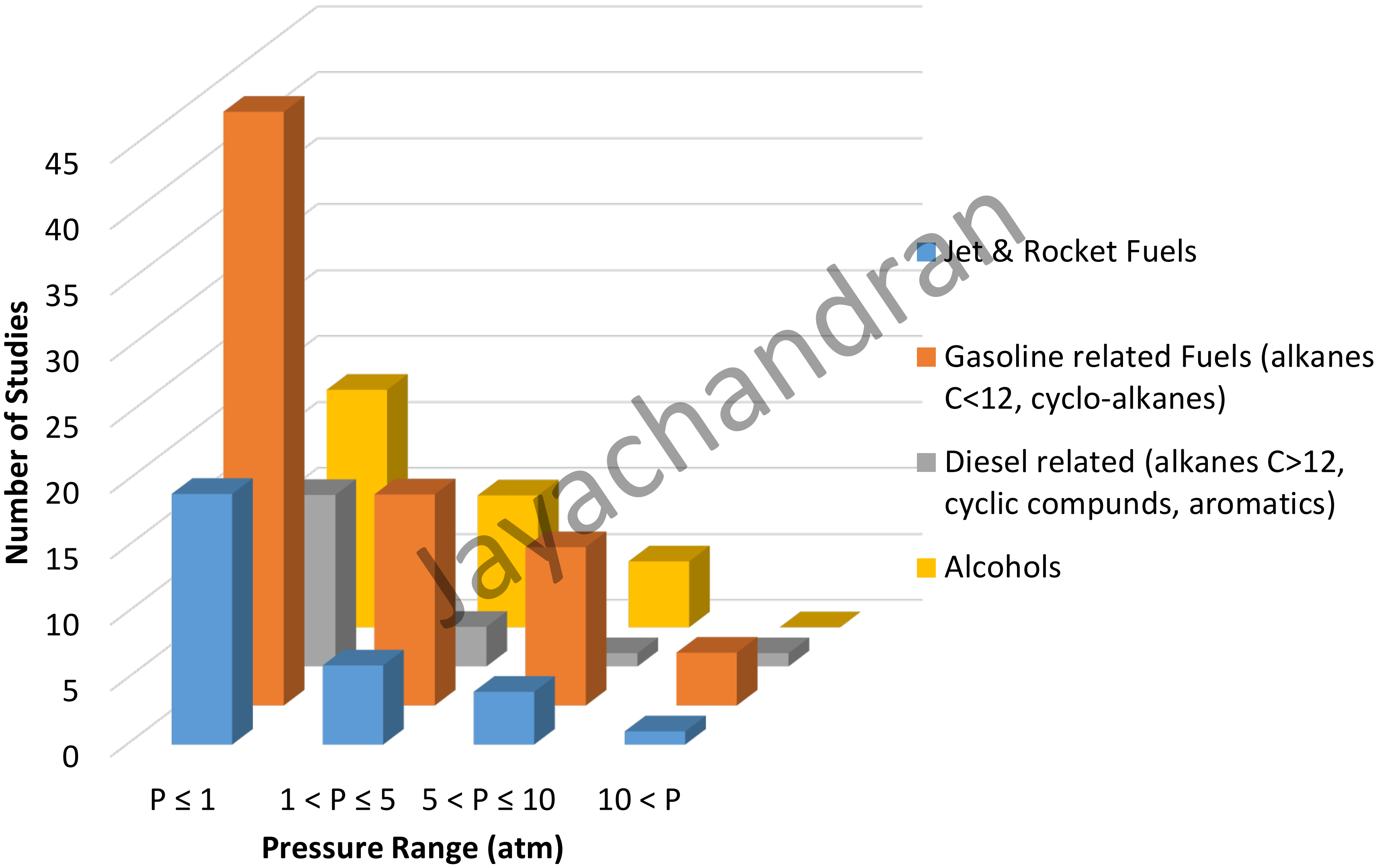


T_u: Unburned mixture temperature

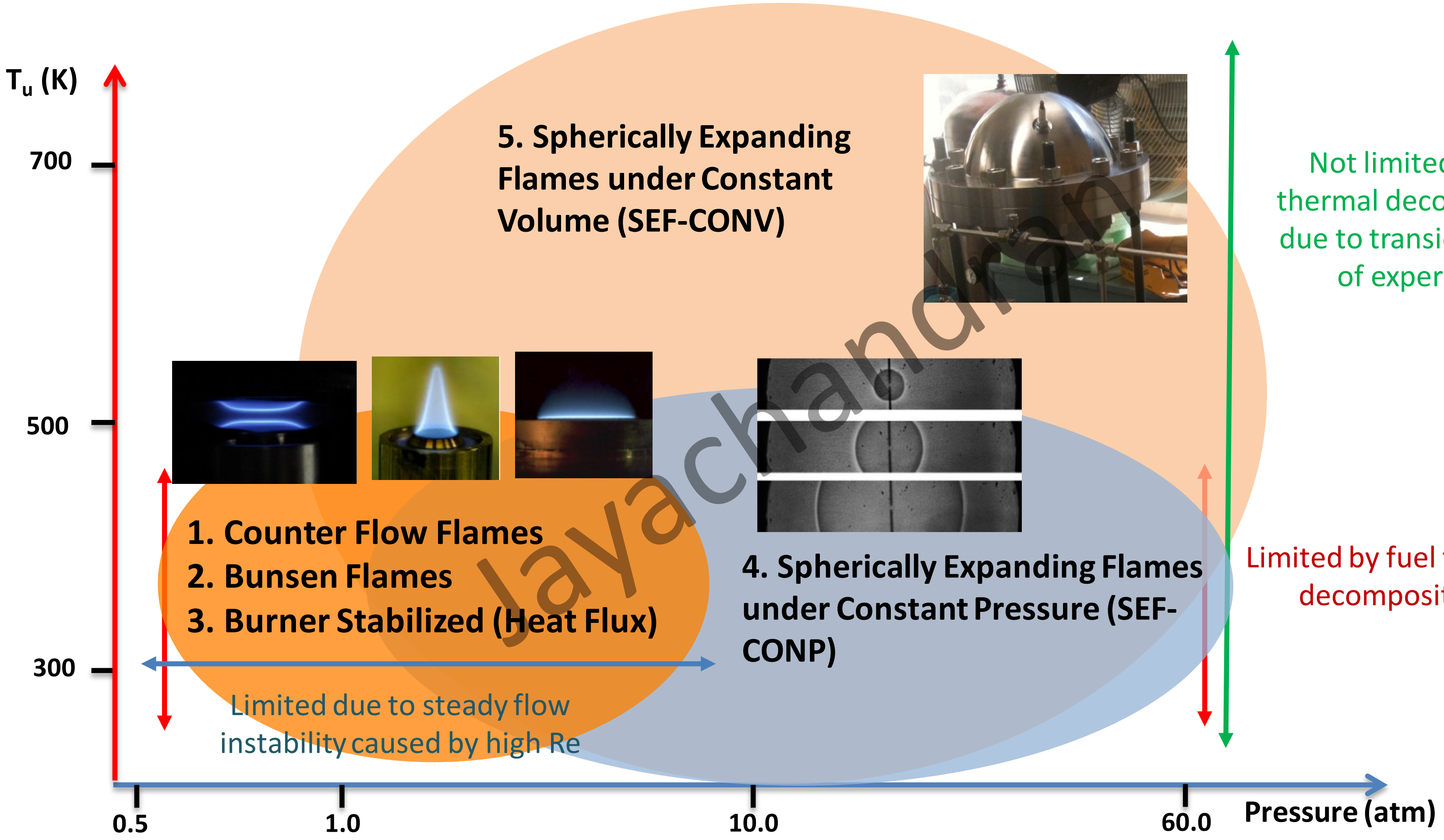
Laminar flame speed studies: light fuels



Laminar flame speed studies: heavy fuels



Legacy experiments for measuring laminar flame speeds



5. Spherically Expanding Flames under Constant Volume (SEF-CONV)

Not limited by fuel thermal decomposition due to transient nature of experiment

1. Counter Flow Flames
2. Bunsen Flames
3. Burner Stabilized (Heat Flux)

Limited due to steady flow instability caused by high Re

4. Spherically Expanding Flames under Constant Pressure (SEF-CONP)

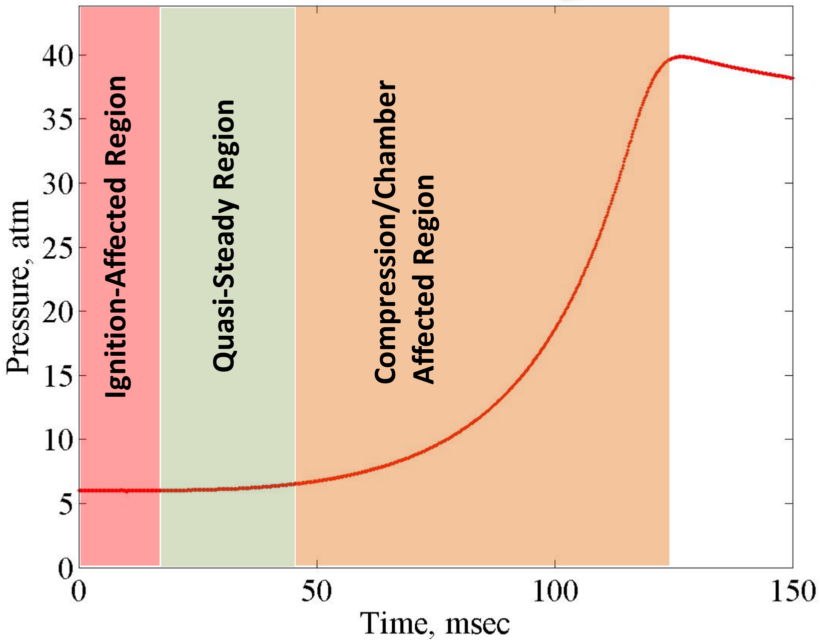
Limited by fuel thermal decomposition

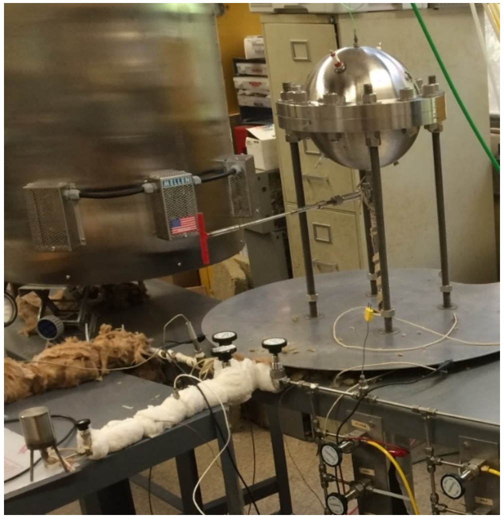
T_u: Unburned mixture temperature

Spherically expanding flame constant-volume method (SEF-CONV)

- Proposed by Lewis and von Elbe[1] in the 1930s
- Advanced by Bradley and Mitcheson[2], Metghalchi and Keck[3], and others

Unburned gas at high pressure and temperature





Example: *n*-C_7H_{16}/oxidizer mixtures Starting at P_o= 8 atm and $T_{u,o}$= 450 K, values of P ~ 50 atm and T_u~ 680 K can be reached.

[1] B. Lewis , G. von Elbe, J. Chem. Phys. 2 (1934) 283–290.

[2] D. Bradley, A. Mitcheson, Combust. Flame 26 (1976) 201-217.

[3] M. Metghalchi , J.C. Keck , Combust. Flame 38 (1980) 143-154.

Not a direct measurement!

- We have to derive flame speeds from pressure vs time recordings
- Assuming that the flame is spherical and the unburned gas is isentropically compressed[1],

$$S_u = \left[\frac{dR_f}{dP} - \left(\frac{R_w^3 - R_f^3}{3R_f^2\gamma_u}\right)\frac{1}{P}\right] \times \frac{dP}{dt}$$

modeled: ***R_f (P)***
→ measure of burned mass fraction

measured: ***P*** **(*t*)**
→ measure of burning rate

- Sources of uncertainty
  - Flame area growth due to cellular instability
  - Influence of flame stretch
  - Accuracy of the ***R_f (P)*** model
  - Effect of transient pressure rise?

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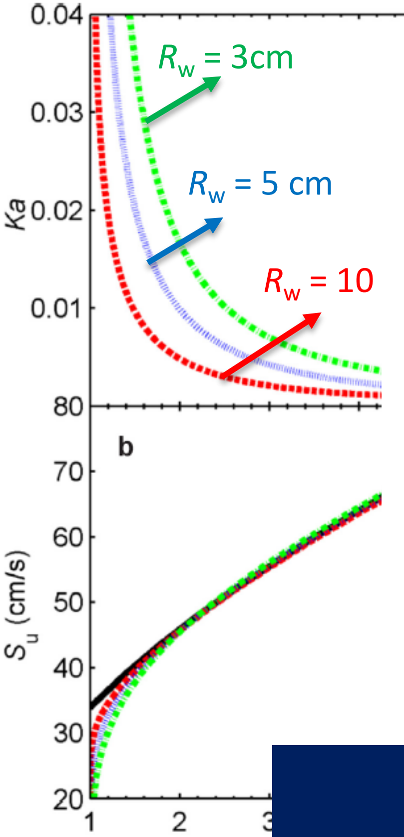
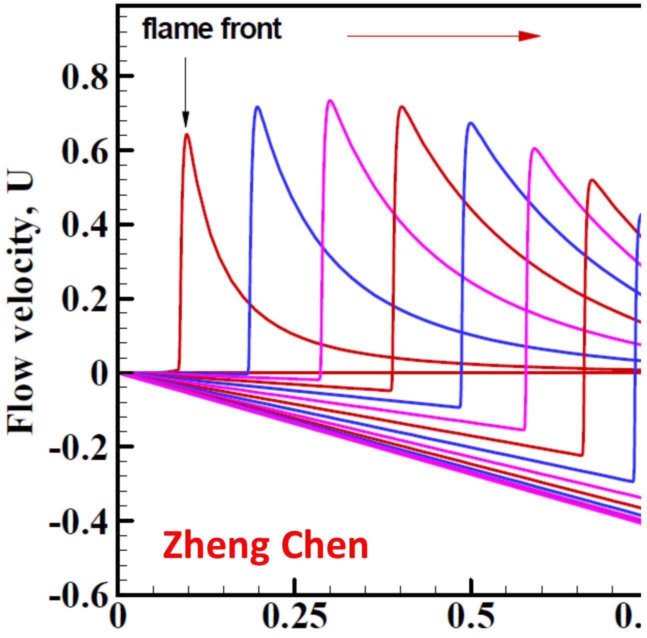
[1] E.F. Fiock, C.F. Marvin, Chem. Rev. 21 (1937) 367-387.

Effect of flame stretch

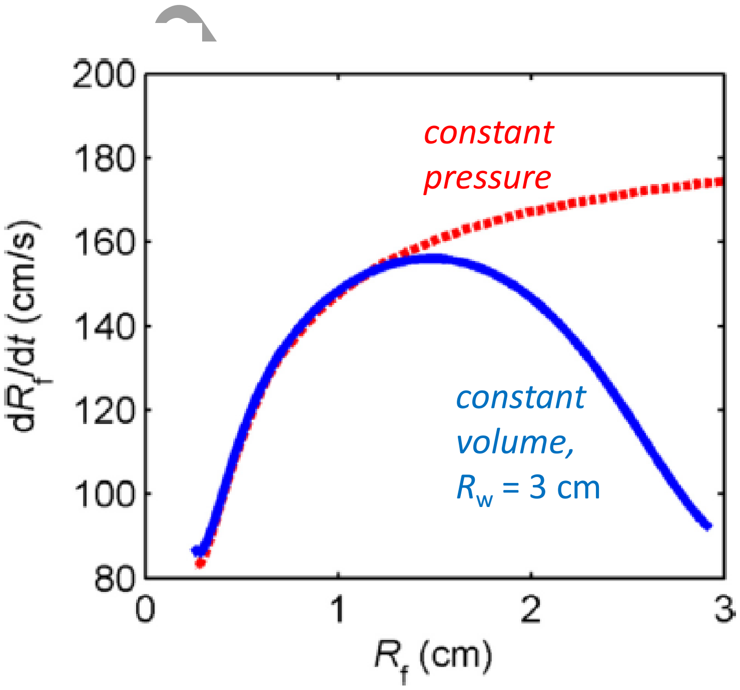
$$Stretch\ Rate = K = \frac{2}{R_f}\frac{dR_f}{dt}$$

$$Karlovitz\ Number = Ka = \frac{characteristic\ time\ scale\ of\ flame}{characteristic\ time\ scale\ of\ stretch} = K\frac{\alpha}{S_u^{\,2}}$$





Zheng Chen



Stretch effects can be neglected for $P/P_o > 2.5$

Accuracy of the $R_f\ (P)$ model

- Linear relationship between fractional pressure rise and burned gas mass fraction
- Thermodynamics-based models: Two zone, Multi-zone
- Hybrid ThermoDynamic-Radiation model (HTDR): includes radiation heat loss from the burned gas

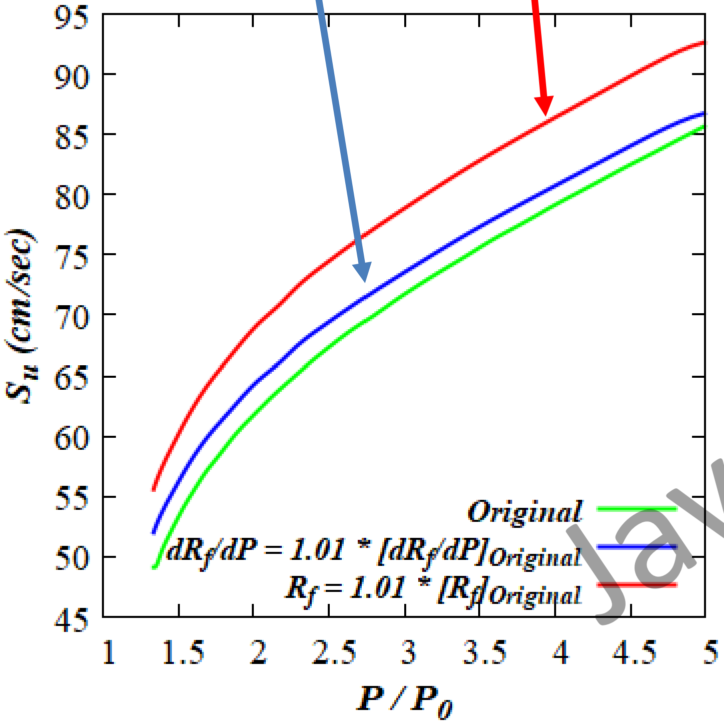
$$S_u = \underbrace{\left[\frac{dR_f}{dP} - \left(\frac{R_w^3 - R_f^3}{3R_f^2\gamma_u}\right)\frac{1}{P}\right]}_{\boxed{\text{modeled: } R_f\ (P)}} \times \frac{dP}{dt}$$

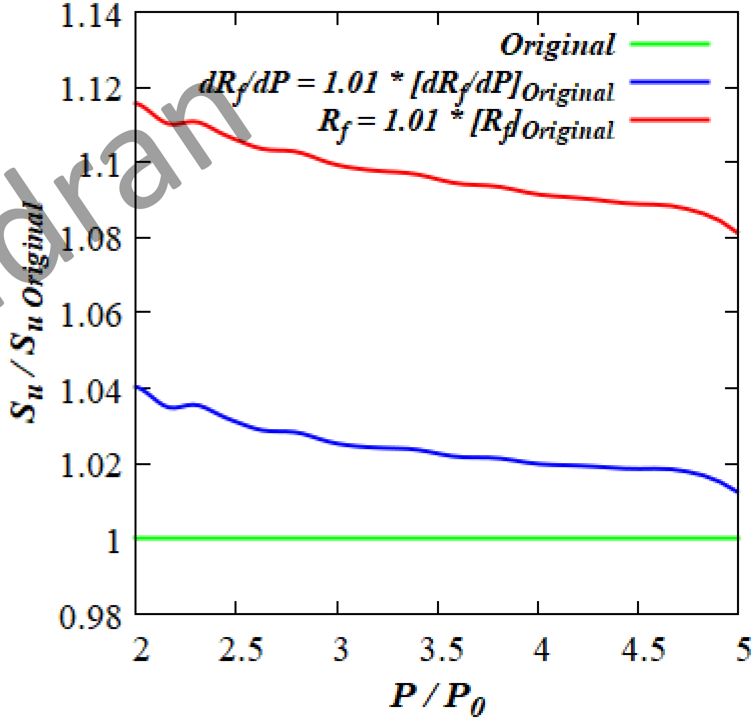
- Perform DNS to obtain $\frac{dP}{dt}$ and $R_f\ (P)$: detailed kinetics and transport

What is the level of accuracy needed for $R_f(P)$?

Accuracy of the $R_f\ (P)$ model

$$S_u = \left[\boxed{\frac{dR_f}{dP}} - \boxed{\left(\frac{R_w^3 - R_f^3}{3R_f^2 \Upsilon_u}\right)\frac{1}{P}}\right] \times \frac{dP}{dt}$$



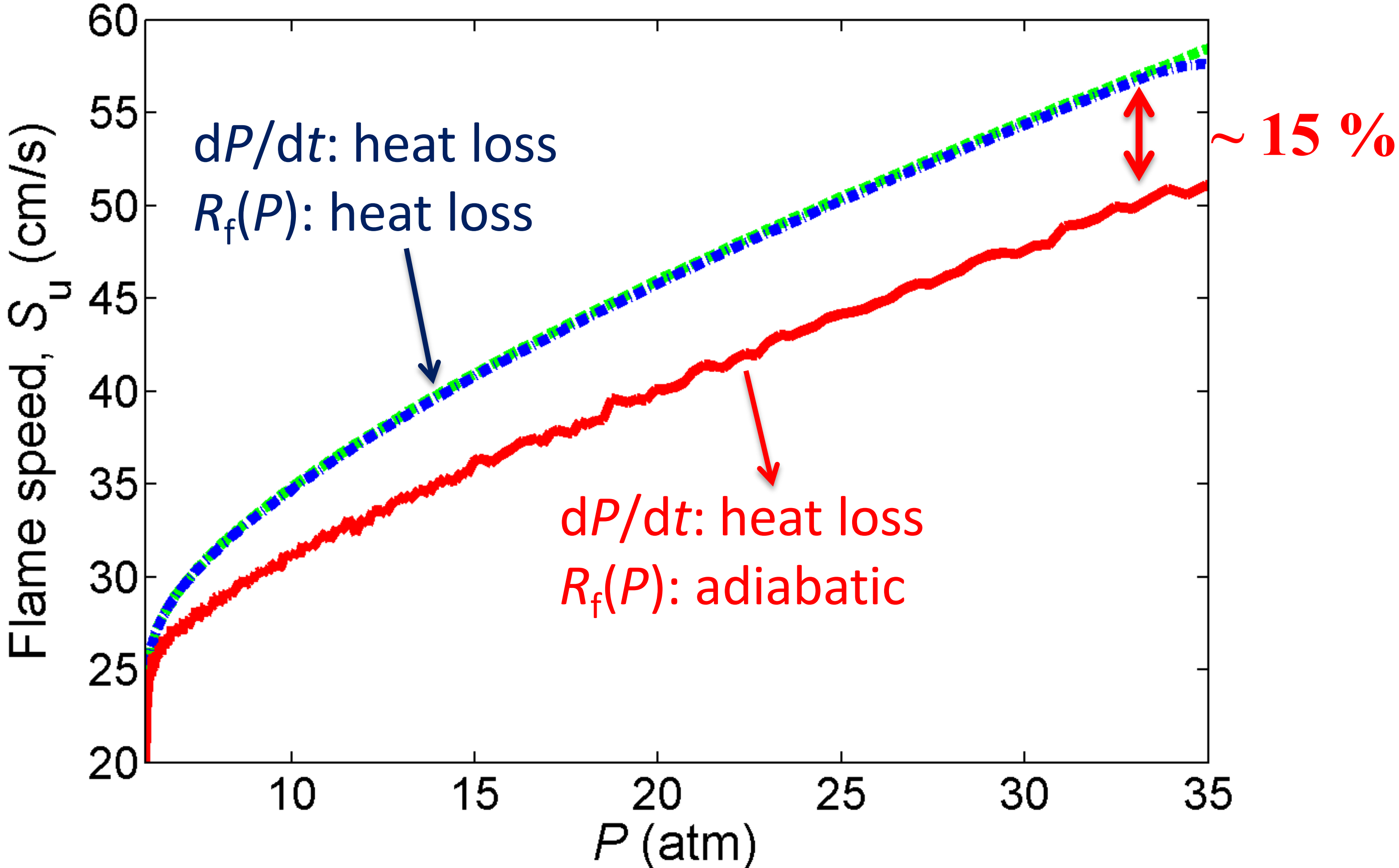


- **Mixture:**
  - **$CH_4/O_2/He$**
  - **$\varphi = 0.8$**
  - **P_o=3atm, T_o=298K**
  - **T_{ad}=2200K**
  - **Mechanism: Lu et al.**

Accuracy of the $R_f\,(P)$ model: case studies

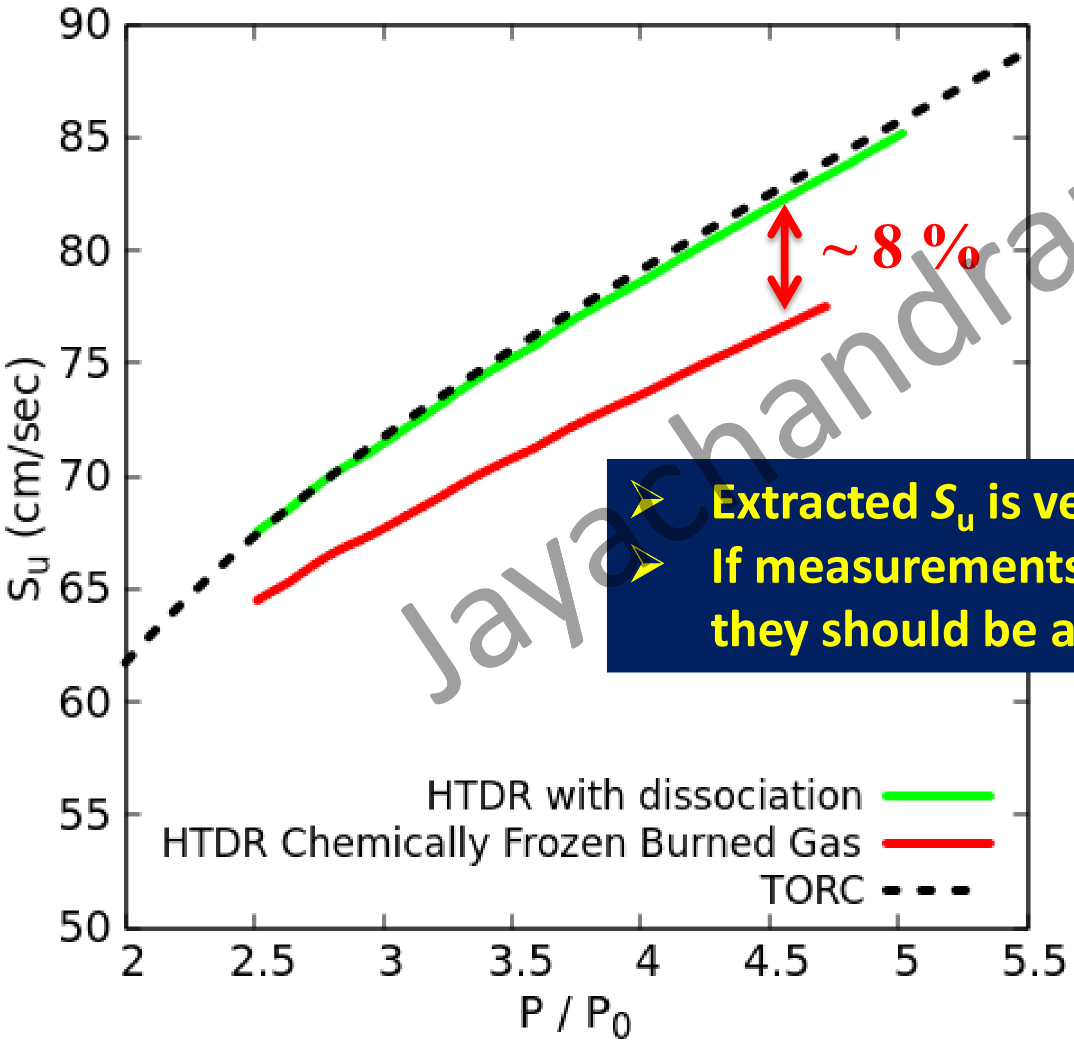
1. Radiation heat loss from the burned gas (continued)

$$S_u = \frac{dR_f}{dt} - \frac{\left(R_w^3 - R_f^3\right)}{3R_f^2\gamma_u P}\frac{dP}{dt}$$



Accuracy of the R_f *(P)* model: case studies

2. Dissociation (evolving thermodynamic state) of burned gas



$$S_u = \frac{dR_f}{dt} - \frac{\left(R_w^3 - R_f^3\right)}{3R_f^2 \gamma_u P} \frac{dP}{dt}$$

- Extracted S_u is very sensitive to R_f*(P)*!!
- If measurements of R_f*(P)* are attempted, they should be accurate to within 1%

- Mixture:
  - CH_4/ O_2/ He
  - *φ* = 0.8
  - *P_o*=3atm, T_o=298K
  - T_{ad}=2200K
  - Mechanism: Lu et al.

Effect of transient pressure rise

- Perform DNS to parametrically investigate the effect of **d*P*/dt** on flame propagation rate

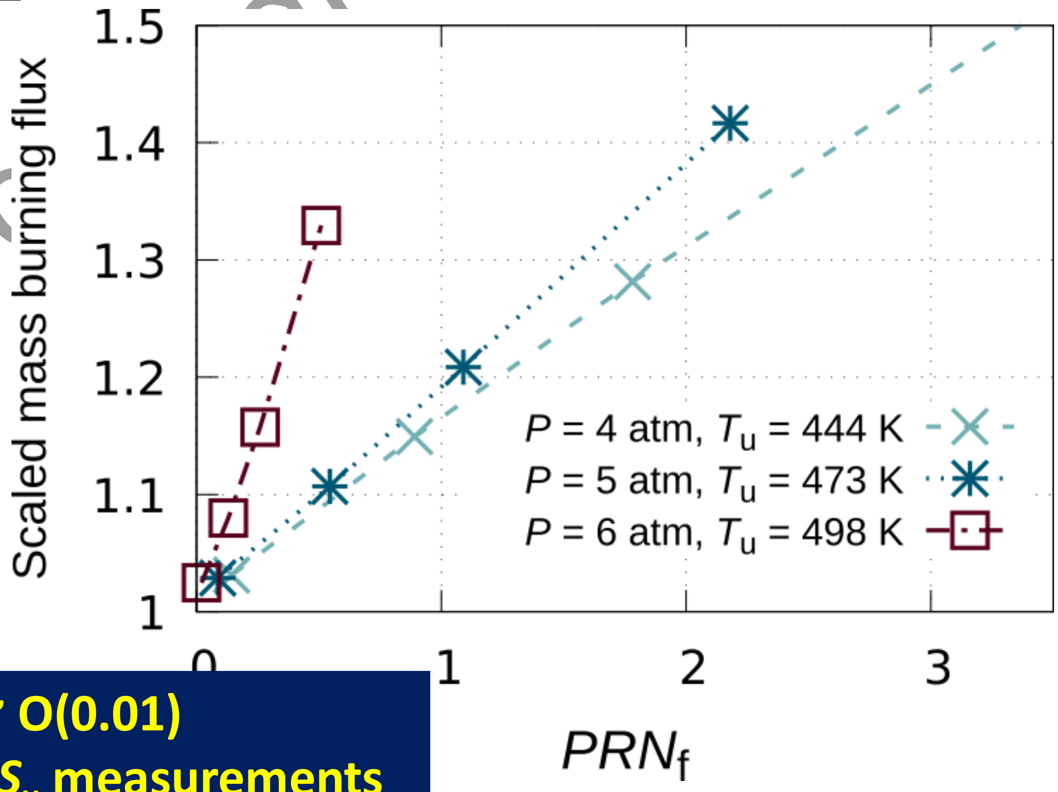
H_2/air
$\phi = 0.6$
$T_u^o = 300$ K
$P_o = 1$ atm

Pressure Rise Number (PRN)

$$PRN_f \equiv \frac{time\ scale\ of\ flame\ propagation}{time\ scale\ of\ pressure\ rise}$$

$$PRN_f \equiv \left(\frac{1}{P}\frac{dP}{dt}\right) t_f$$

$$t_f \equiv \left(\frac{l_f^o}{S_u^o}\right)$$



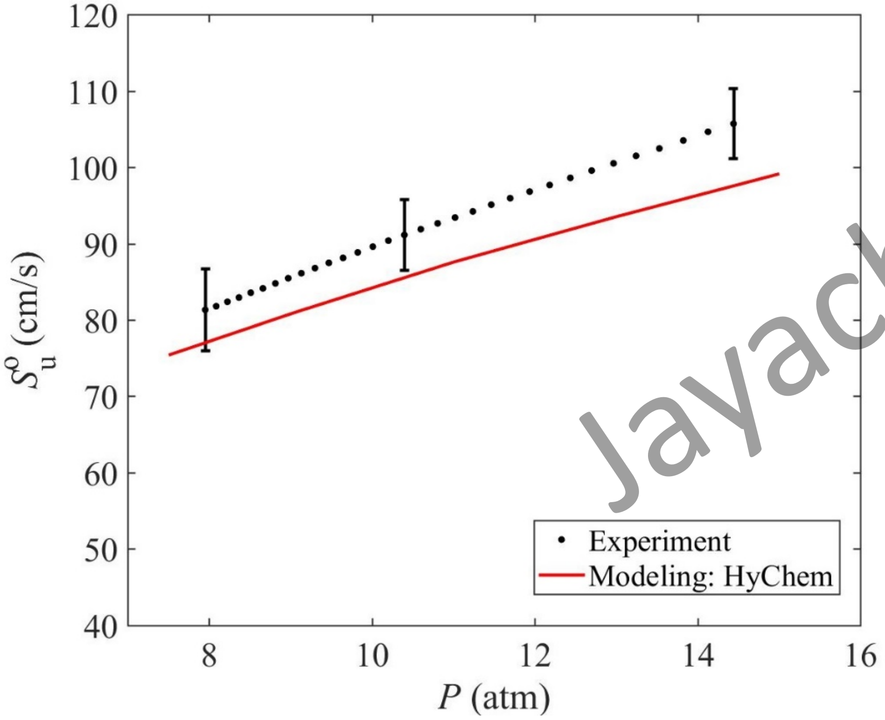
- **In SEF-CONV experiments, PRN ~ O(0.01)**
- **Negligible influence of d*P*/dt on S_u measurements**

Experimental and Modeling Results

JetA/oxidizer mixtures

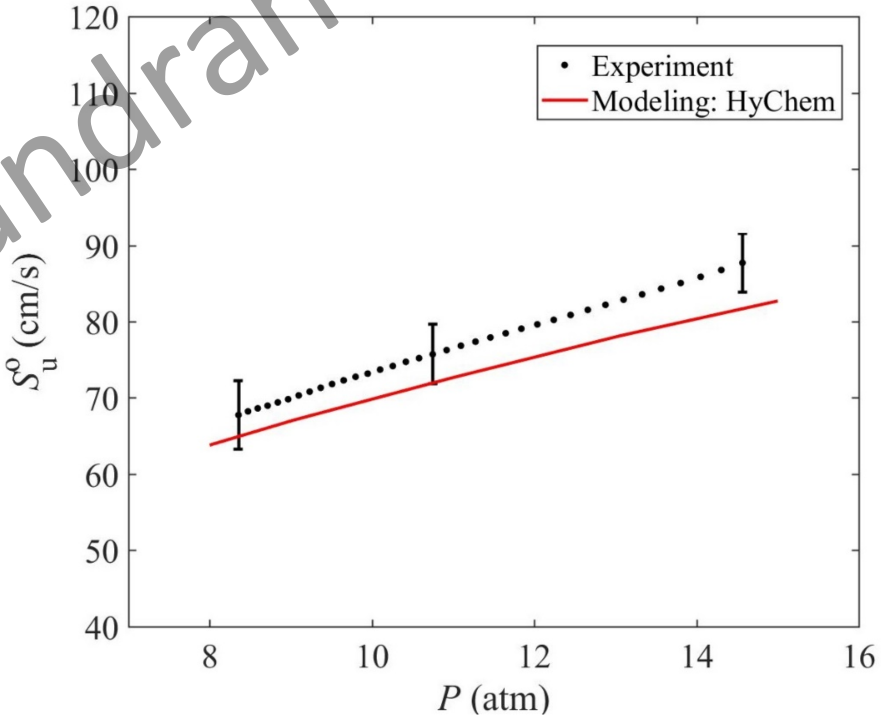
$\phi = 0.9$

$0.9C_{11.37}H_{21.87} + 16.84O_2 + 39N_2 + 58.5He$



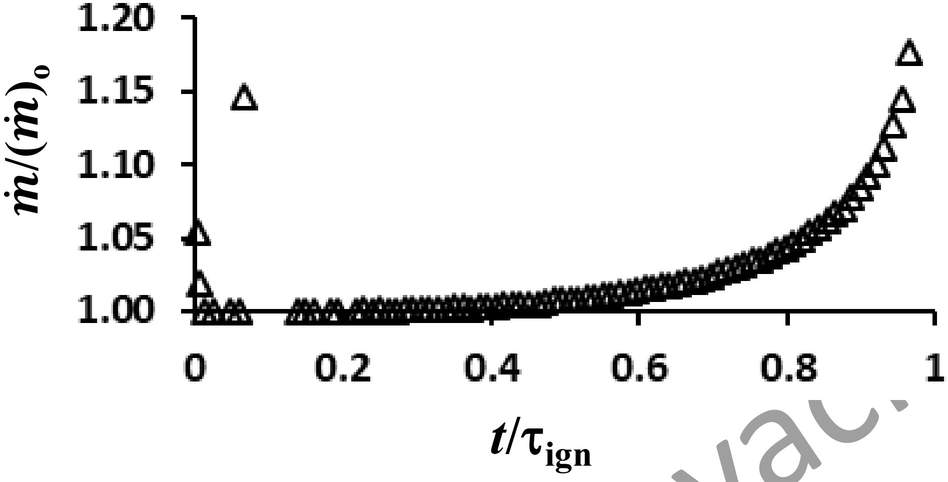
$\phi = 1.05$

$1.05C_{11.37}H_{21.87} + 16.84O_2 + 44.75N_2 + 61.13He$

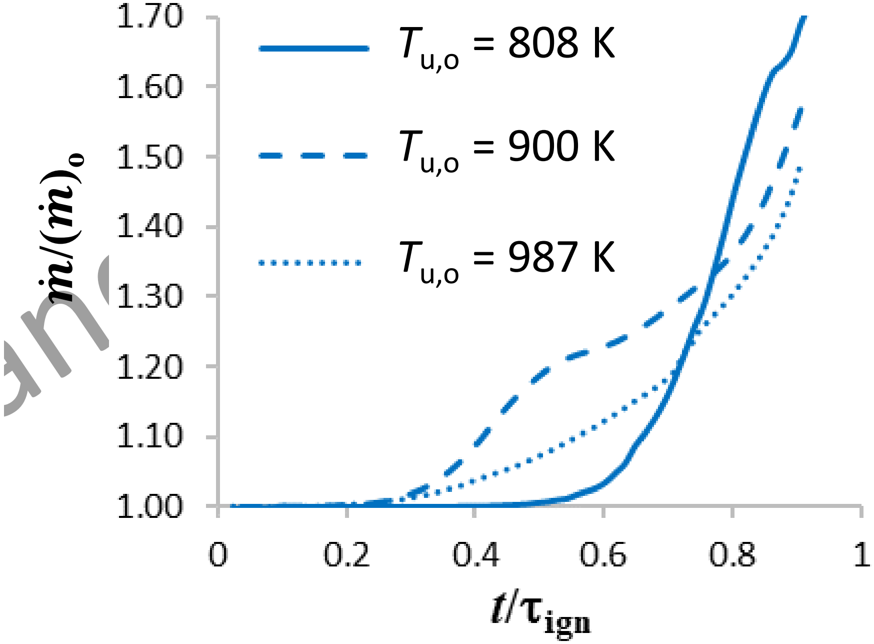


Flame propagating into a reacting mixture

$H_2/O_2/N_2$
P = 55 atm
$T_{u,o}$ = 900 K



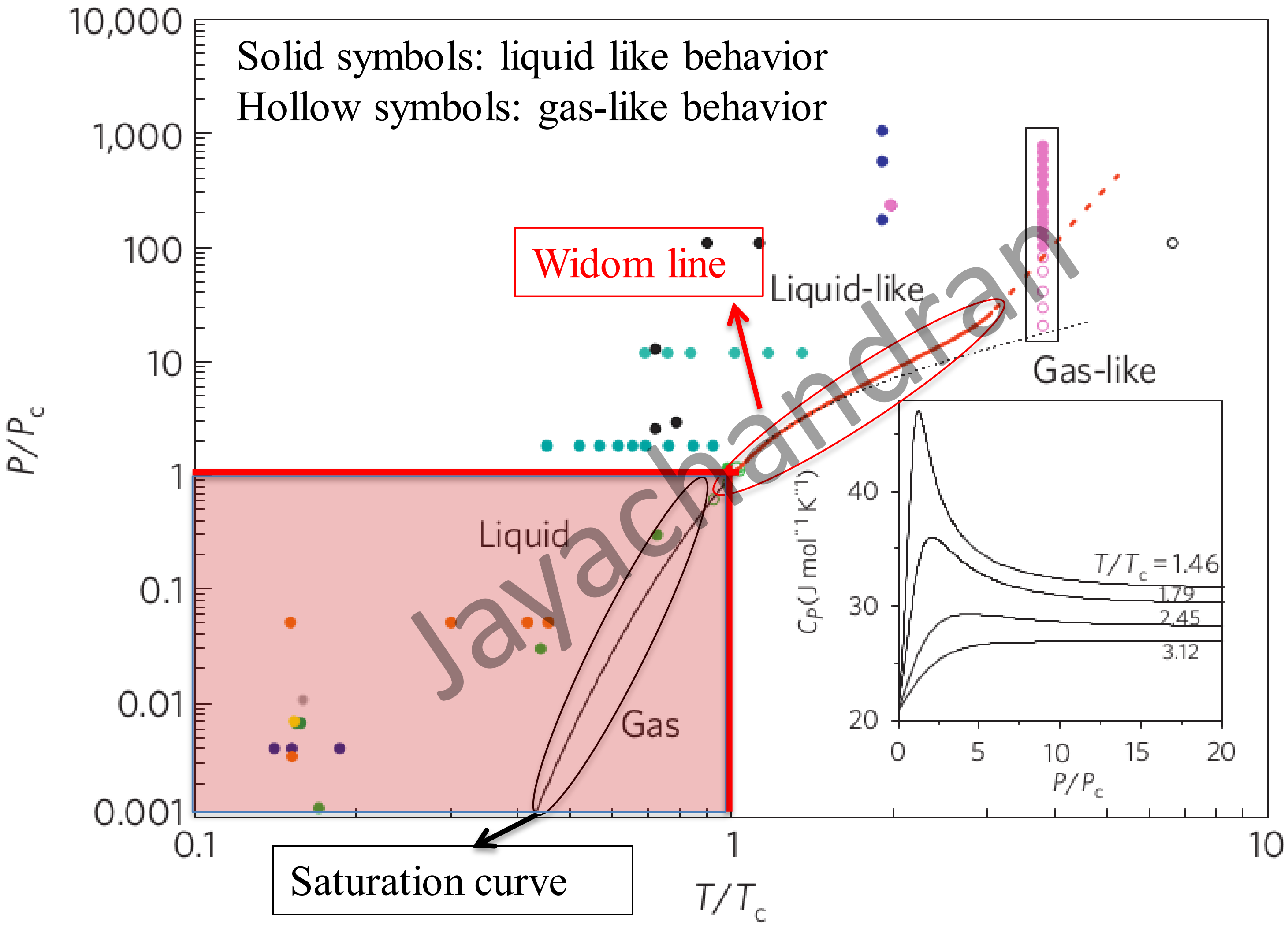
n-C_7H_{14}/air mixture
P = 40 atm



- Unique steady-state solution does not exist: no unique eigen value
- Very important phenomena but interpreting experimental data requires advanced diagnostics and computational capabilities

A. Ansari, J. Jayachandran, F.N. Egolfopoulos, Pro. Combust. Inst. 37 (2019) 1513-1520.

Physics at high pressures



Solid symbols: liquid like behavior

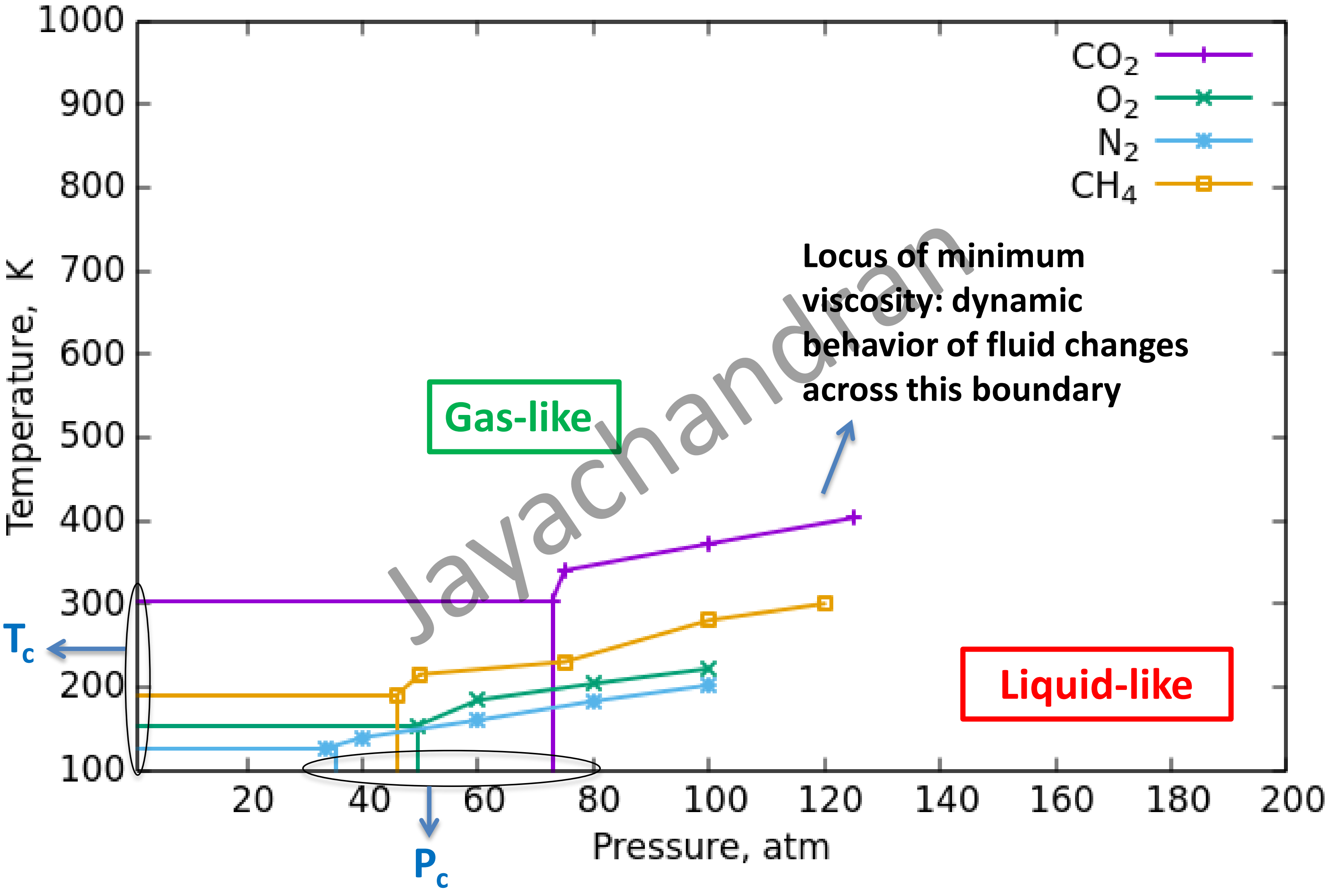
Hollow symbols: gas-like behavior

Widom line

Saturation curve

Simeoni et al., The Widom line as the crossover between liquid-like and gas-like behavior in supercritical fluids, Nature Physics, vol 6 (2010).

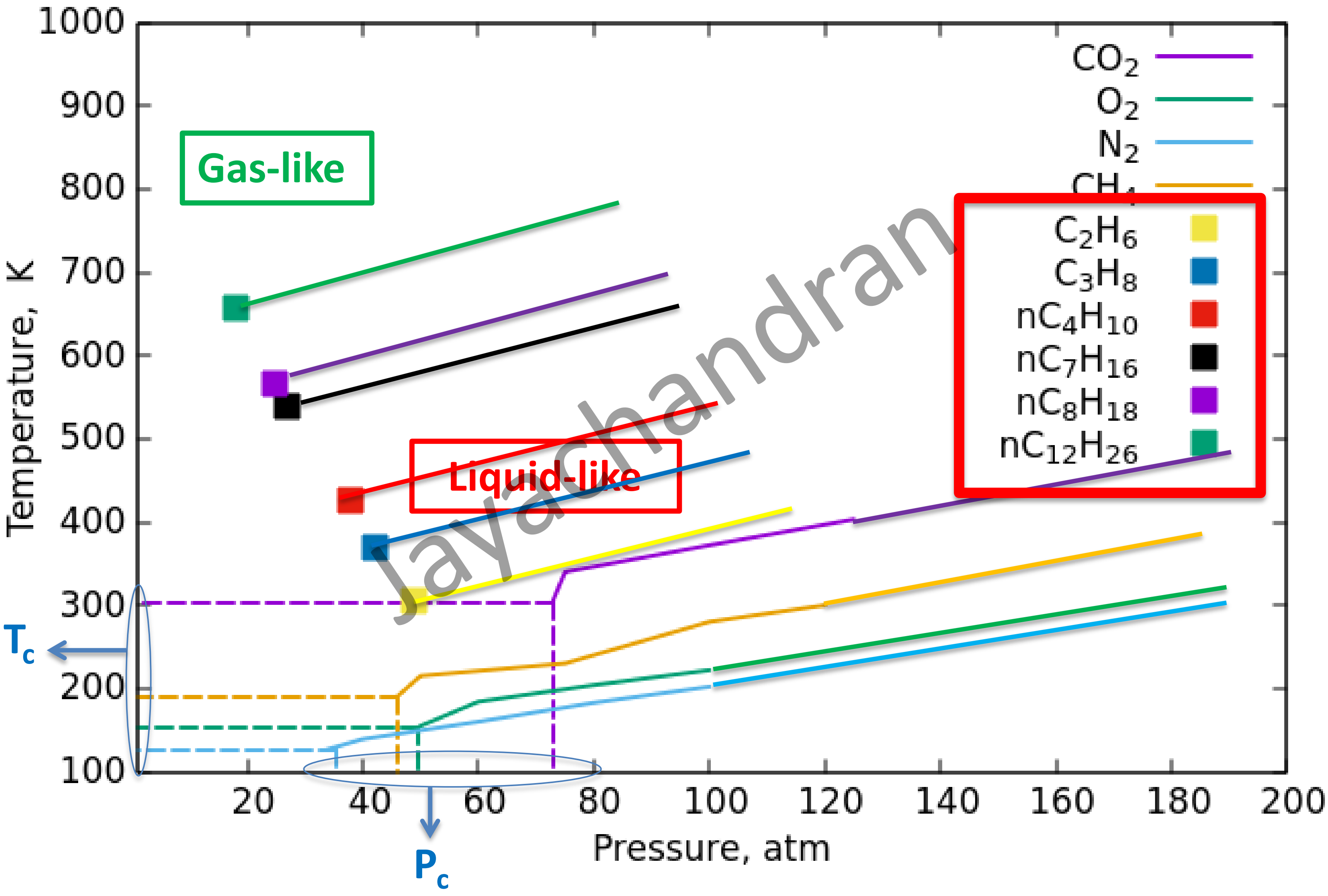
Engine conditions vs thermodynamic conditions



Locus of minimum viscosity: dynamic behavior of fluid changes across this boundary

NIST chemistry Webbook: Thermophysical properties of fluid systems

Engine conditions vs thermodynamic conditions



Engine conditions vs thermodynamic conditions