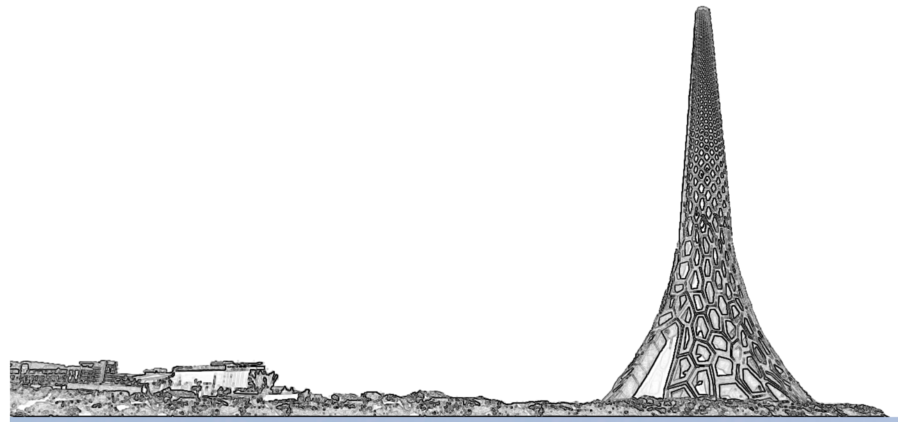
H_2 week in Toulouse, February 26th-29th 2024

Running high-pressure experiments with hydrogen:

challenges, flame stabilization, diagnostics opportunities

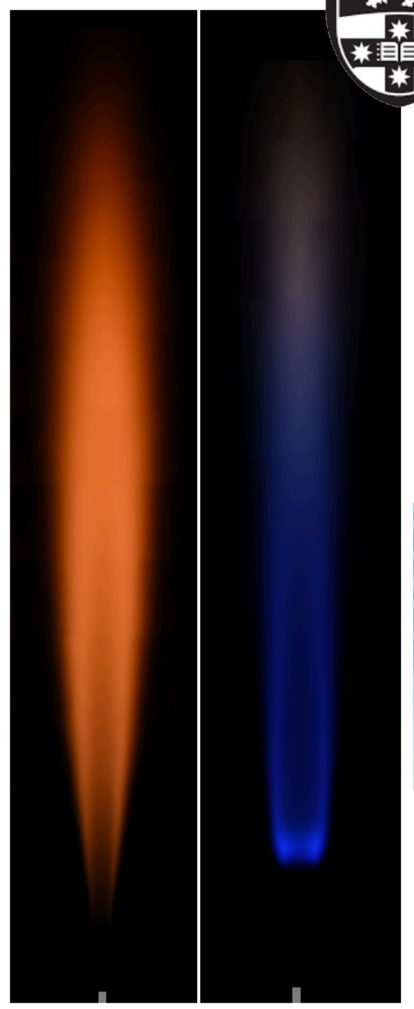
Thibault F. Guiberti

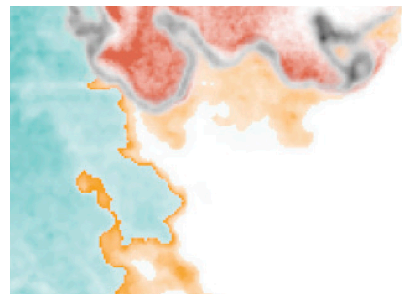


High pressure turbulent flames at KAUST

Non-premixed flames

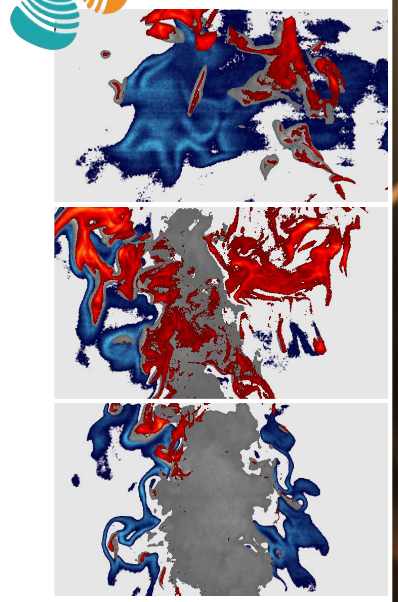
CH_4 & C_2H_6
up to 10 bar and
Re = 50,000





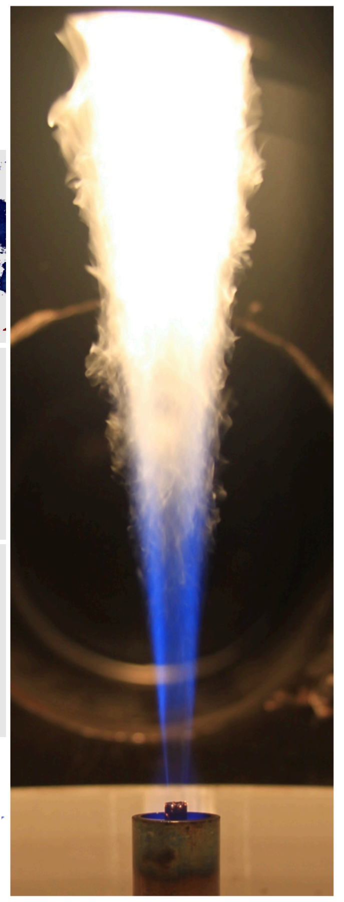
Raman/OH/CH2O

Stabilization



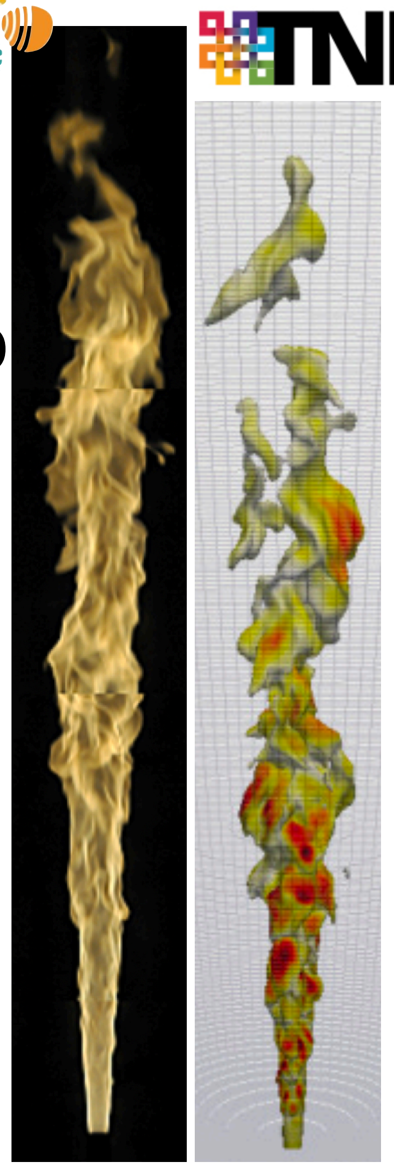
OH/PAH/LII

C_2H_4-N_2
up to 7 bar and
Re = 50,000



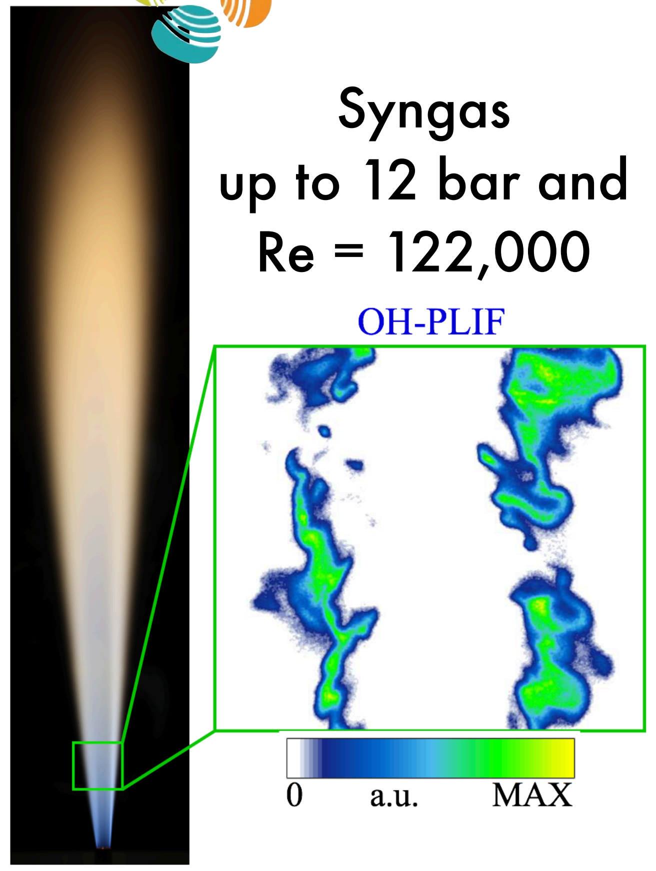
Soot

NH_3-H_2-N_2
up to 5 bar
Re = 11,200



LES

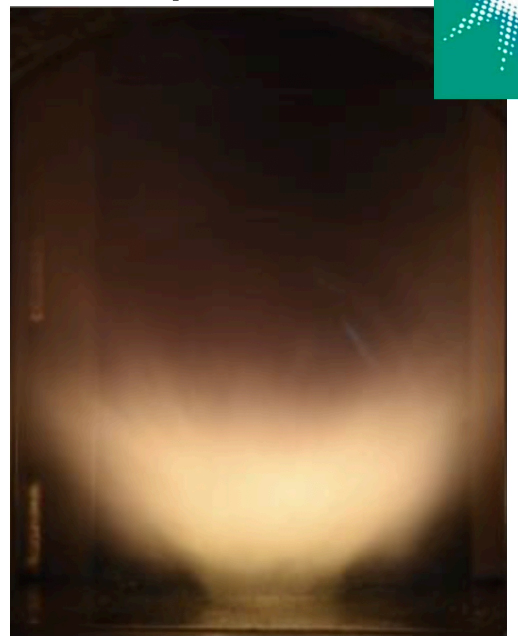
Syngas
up to 12 bar and
Re = 122,000



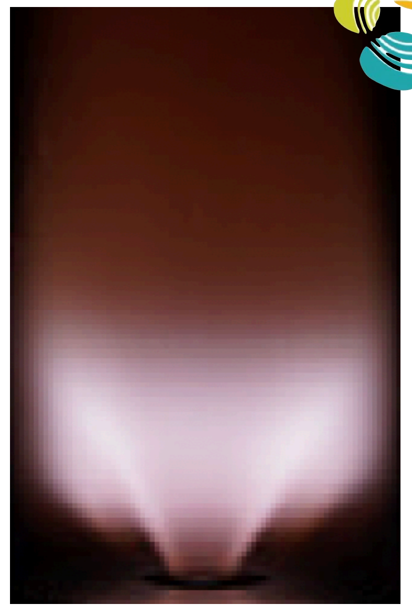
Structure

Premixed flames

NH_3-H_2
up to 5 bar

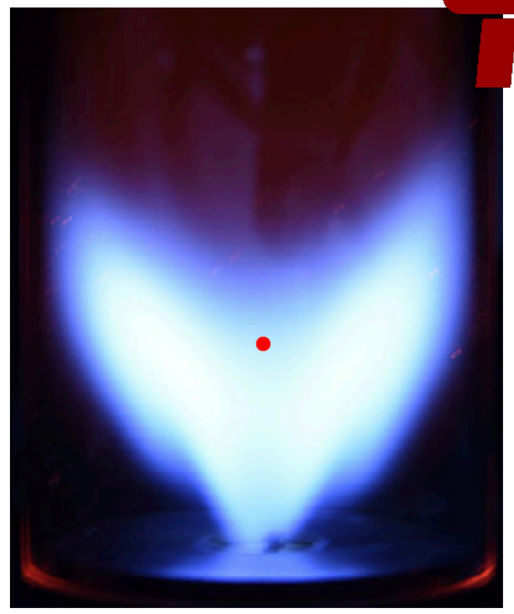


NH_3-CH_4
up to 5 bar

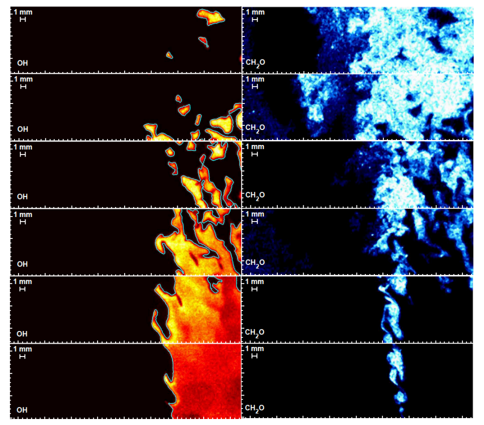


Ammonia blends

CH_4 & C_3H_8
up to 5 bar and
P = 20 kW



Flame dynamics

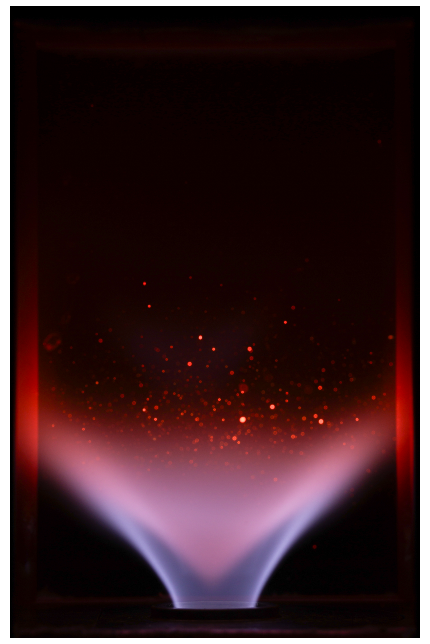


OH CH_2O

CH_4
up to 3 bar and
Re = 170,000

Blow-off

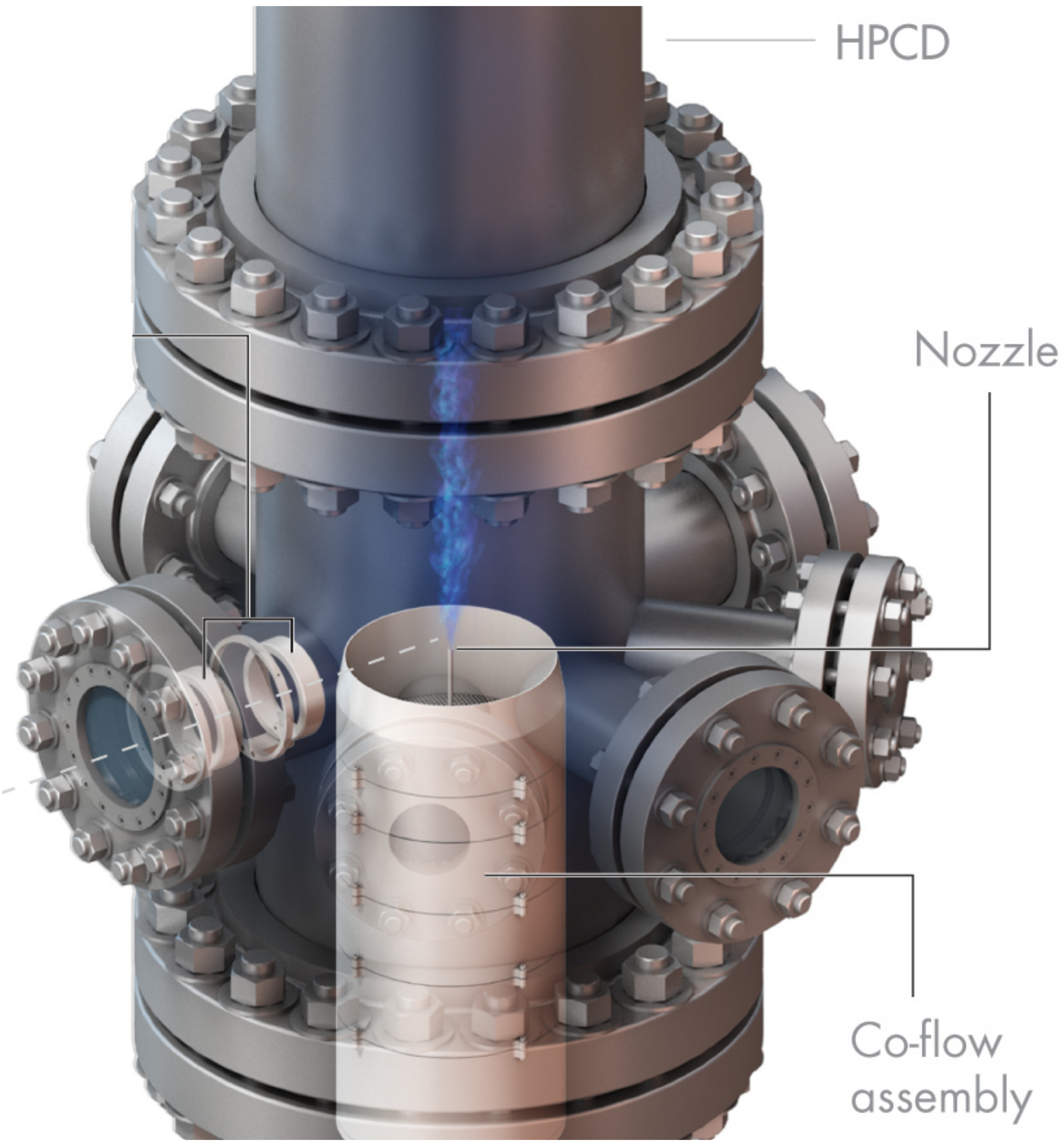
H_2
up to 10 bar



Stabilization

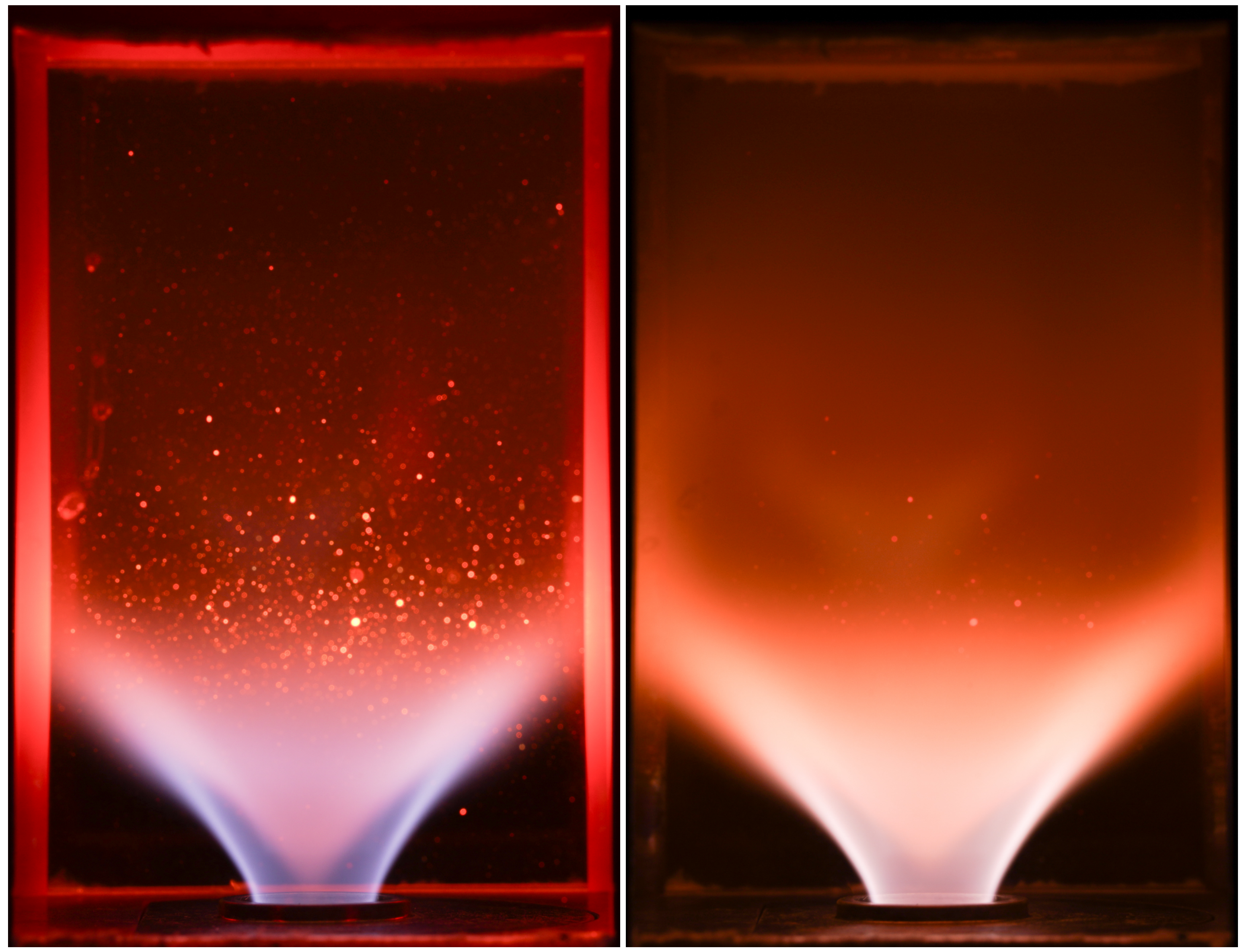
High pressure turbulent H_2 flames at KAUST

H_2-N_2 non-premixed jet flames
up to 12 bar
up to Re = 83,000



H_2-air dual swirl flames

4 bar | 10 bar

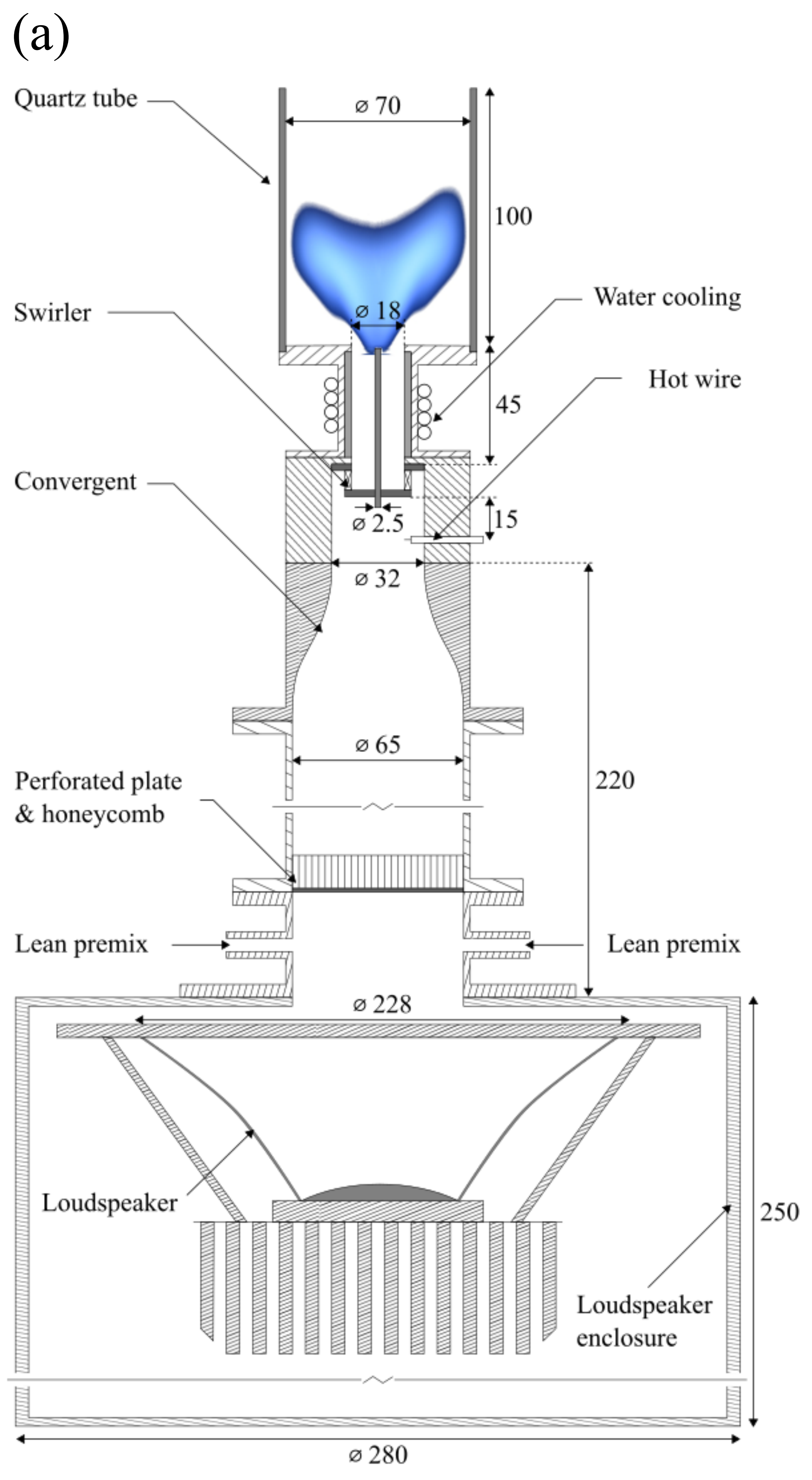


HYLON-KAUST burner

These flames have in common the non-premixed nature of their injection system

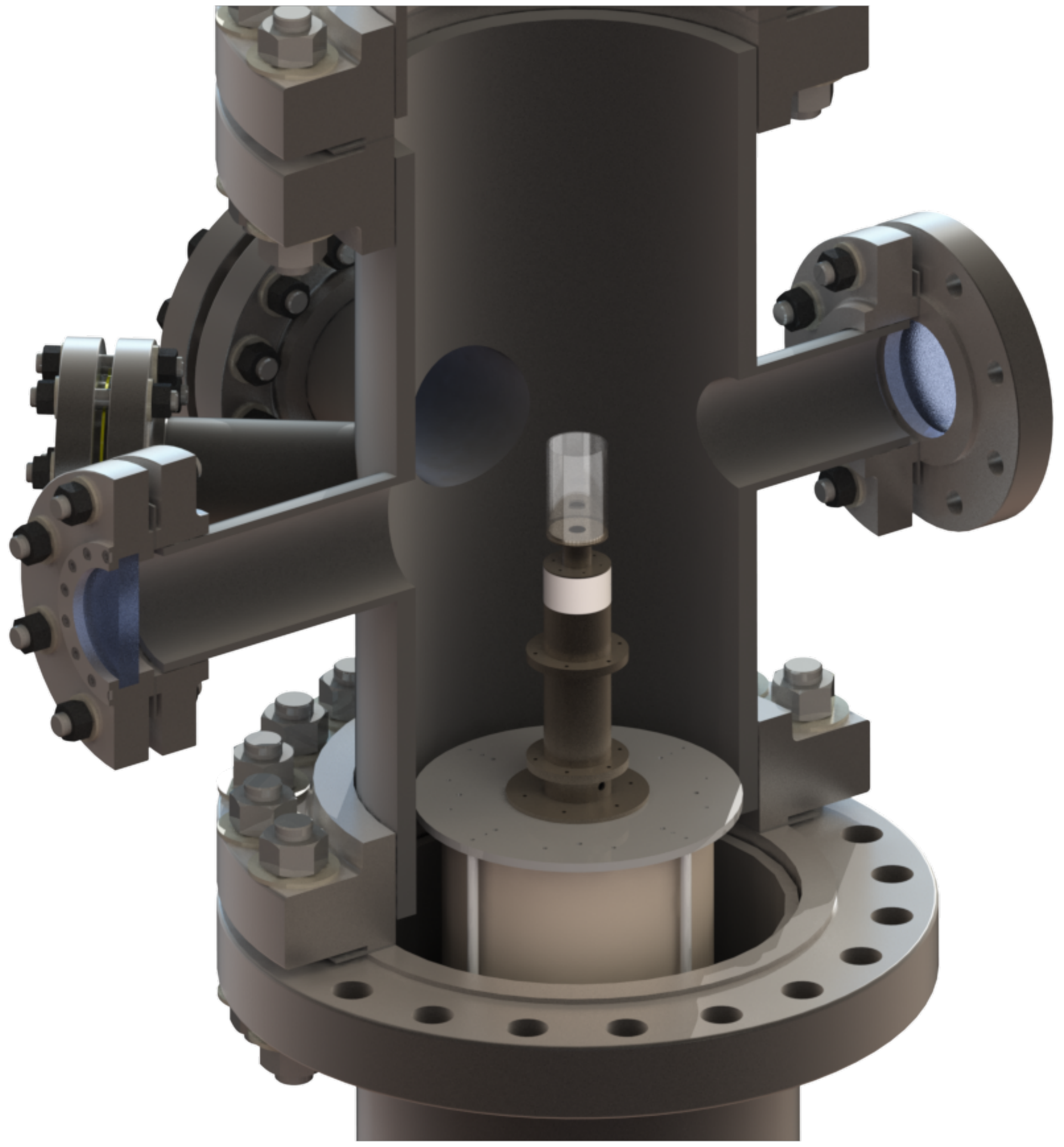
The dreaded flashback...

During FTF measurements in premixed CH_4/C_3H_8-air flames at 5 bar:



Di Sabatino et al. Combust. Flame 2018(193)

(b)



HPCD

Failure of the plenum screws

Deformation of the aluminum rim

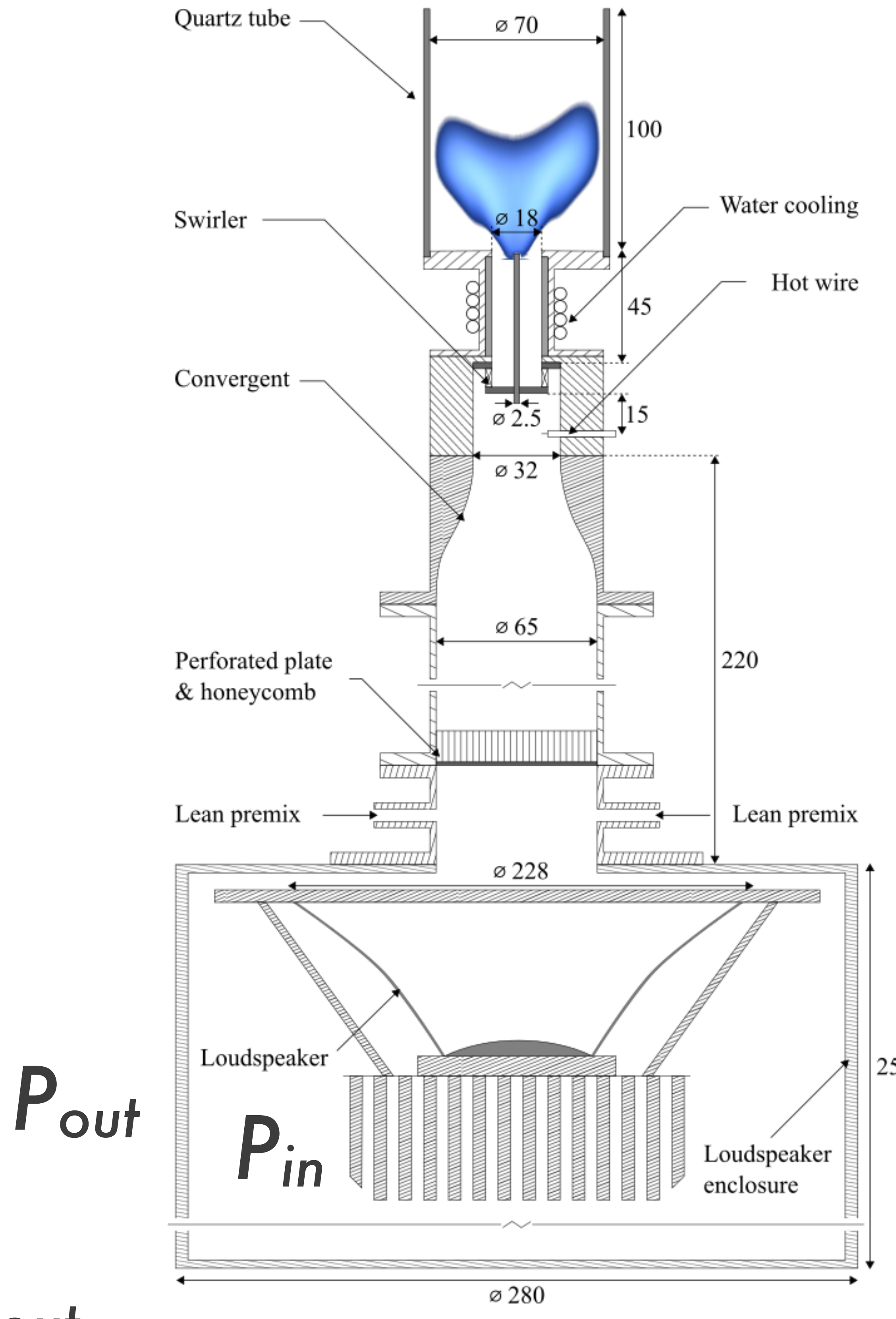
At pressure the severity of the damages due to flashback increase!

The dreaded flashback...

At pressure the severity of the damages due to flashback increase!

Deflagration @ 1 bar for stoichiometric CH_4-air: $\Delta P \simeq 1 \text{ bar} \times (2225K/300K - 1) = 6.4 \text{ bar}$

Deflagration @ 5 bar for stoichiometric CH_4-air: $\Delta P \simeq 5 \text{ bar} \times (2257K/300K - 1) = 32.6 \text{ bar}$



Deflagration @ 1 bar for stoichiometric H_2-air: $\Delta P \simeq 6.9$ bar

Deflagration @ 5 bar for stoichiometric H_2-air: $\Delta P \simeq 35.4$ bar

This assumes an adiabatic flashback process

This also assumes that expanded gases do not escape during flashback

- H_2 flashbacks are more severe due to the larger flame speed

$$\Delta P = P_{in} - P_{out}$$

The dreaded flashback...

Consequences of flashback may be even more dramatic if transition to detonation occurs

Detonation @ 1 bar for stoichiometric CH_4-air: $\Delta P \simeq$ 17.1 - 1 bar = 16.1 bar

Detonation @ 5 bar for stoichiometric CH_4-air: $\Delta P \simeq$ 87.1 - 5 bar = 82.1 bar

Very unlikely to occur

Detonation @ 1 bar for stoichiometric H_2-air: $\Delta P \simeq$ 15.5 - 1 bar = 14.5 bar

Detonation @ 5 bar for stoichiometric H_2-air: $\Delta P \simeq$ 79.3 - 5 bar = 74.3 bar

Detonation @ 10 bar for stoichiometric H_2-air: $\Delta P \simeq$ 160.0 - 10 bar = 150.0 bar

cearun.grc.nasa.gov

The dreaded flashback...

For a detonation to occur, suitable conditions must be met

This includes providing enough space for detonation cells to develop

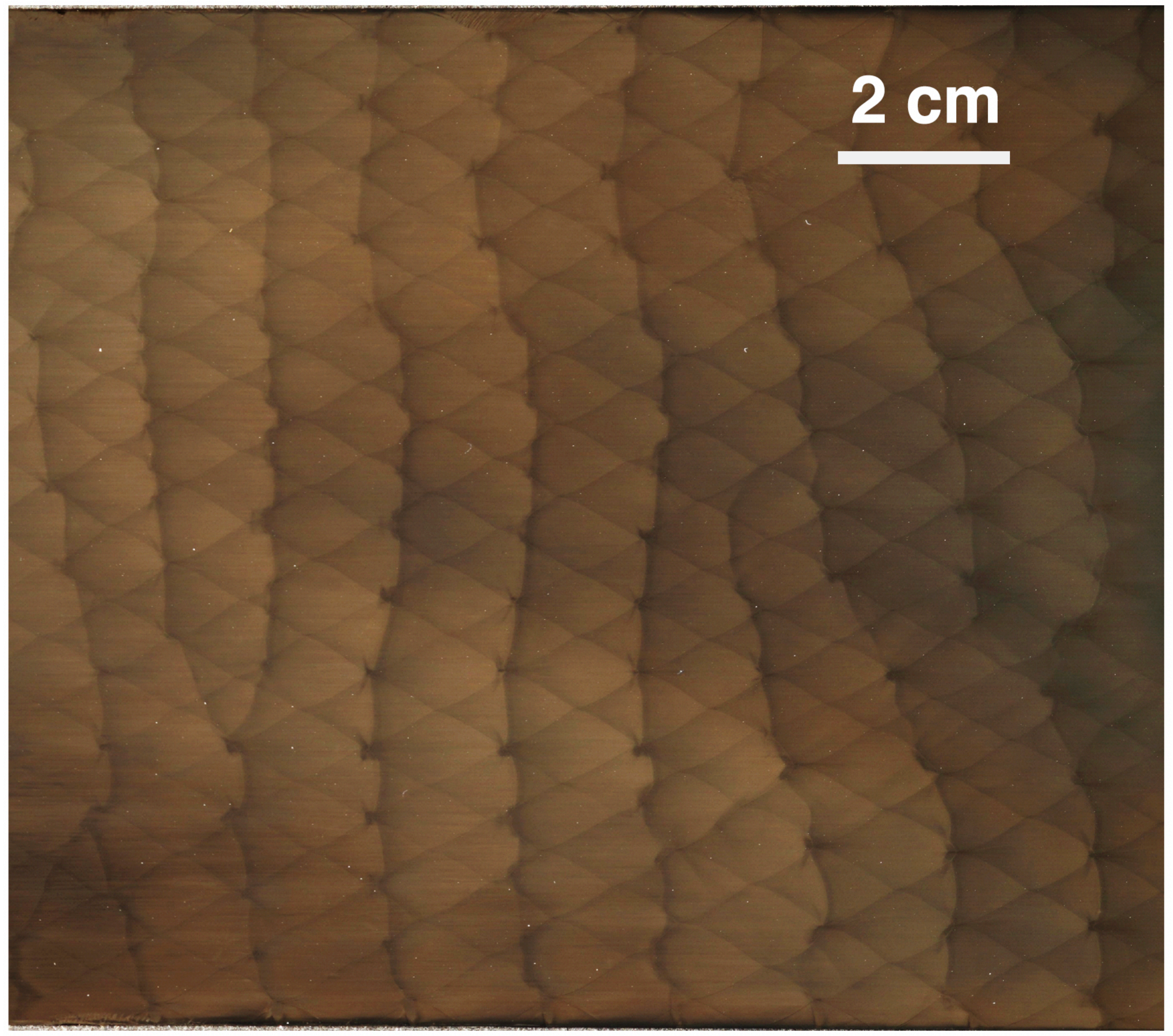
approx. cell width @ 293 K	1 bar	5 bar	10 bar
CH_4-air $\phi = 1$	300 mm	N.A.	N.A.
H_2-air $\phi = 1$	10 mm	5 mm	3 mm
H_2-air $\phi = 0.65$	40 mm	9 mm	8 mm

Kaneshige & Sheperd Detonation database 1999

Curtis A. Babbie Thesis 2015

Soot foil

$2H_2$-O_2-3.76Ar @ 20 kPa & 293 K

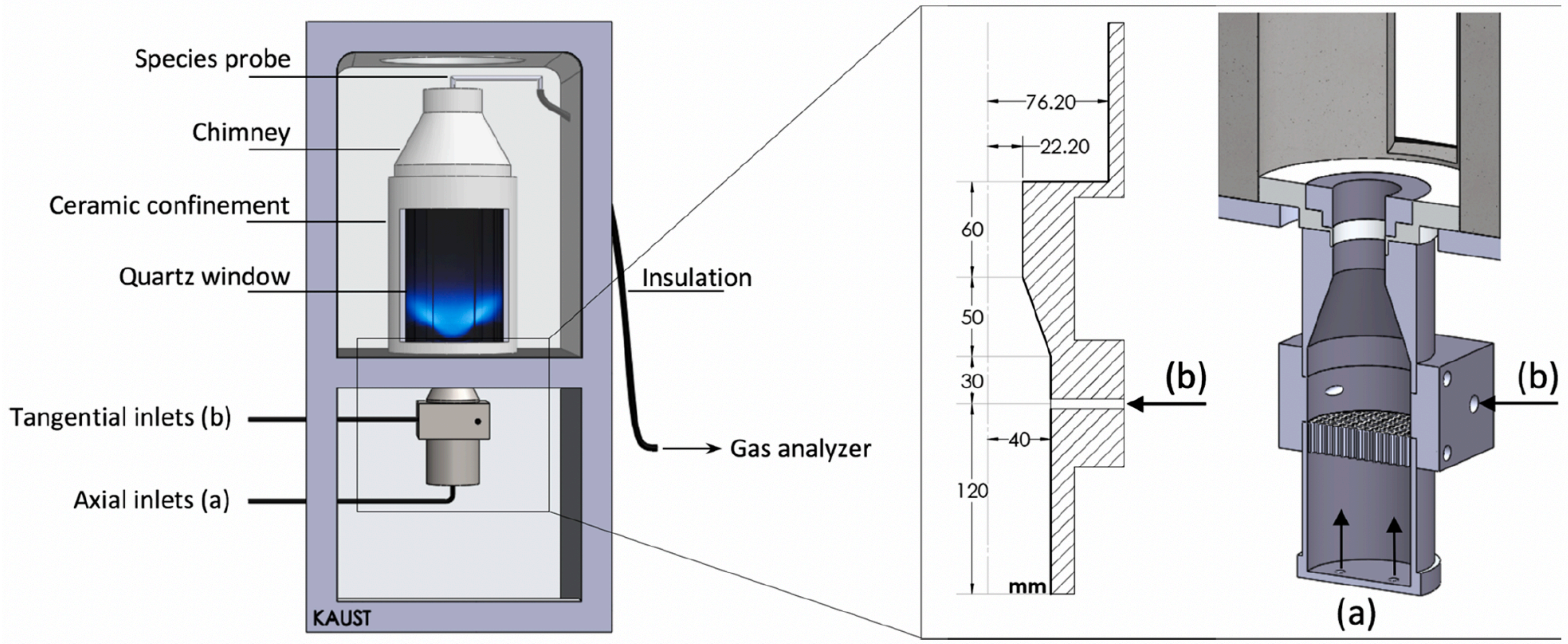


Alicherif et al. Combust. Flame (under review)

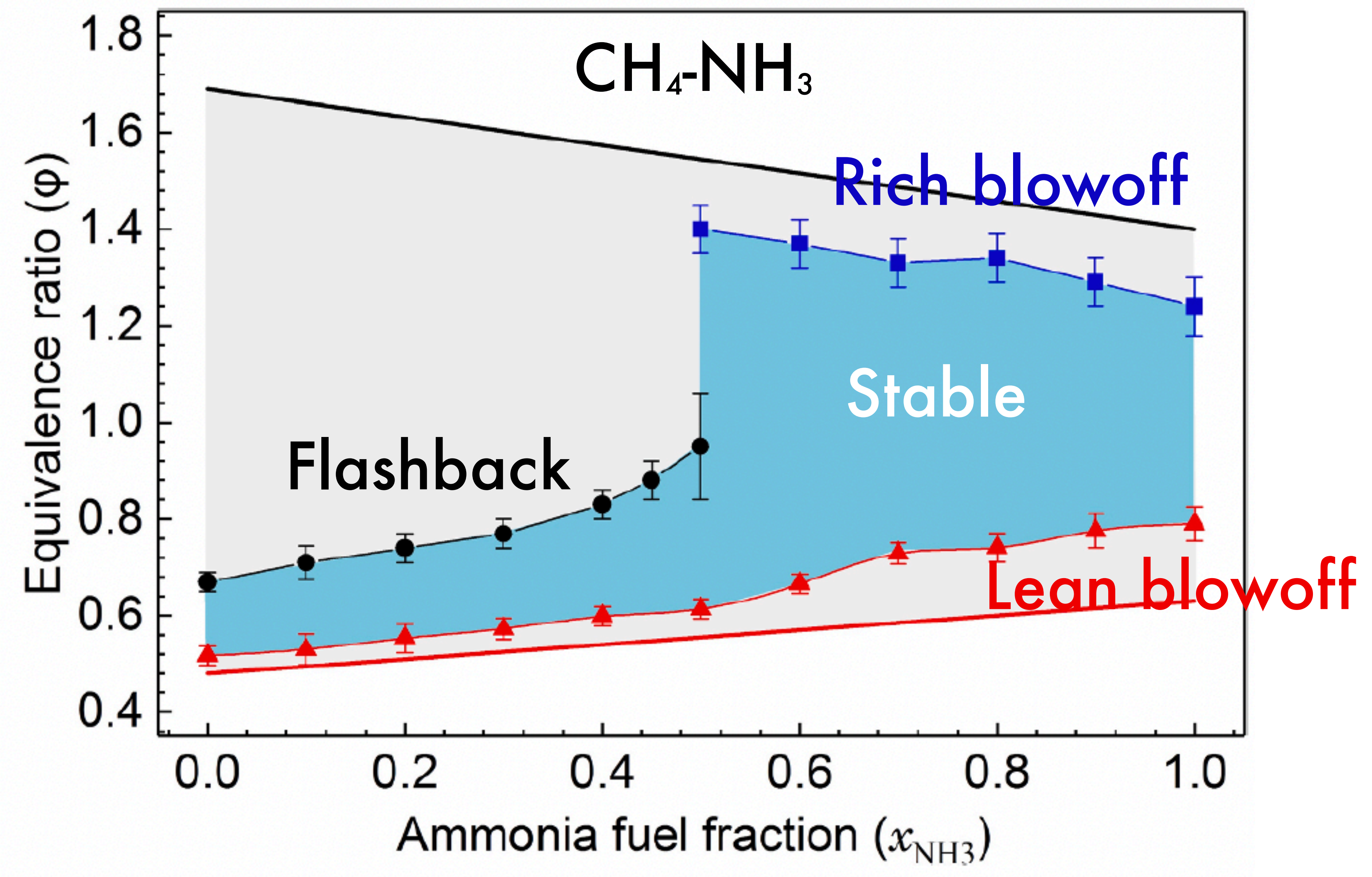
In case of flashback, detonation may occur within the burner for premixed H_2-air mixtures...

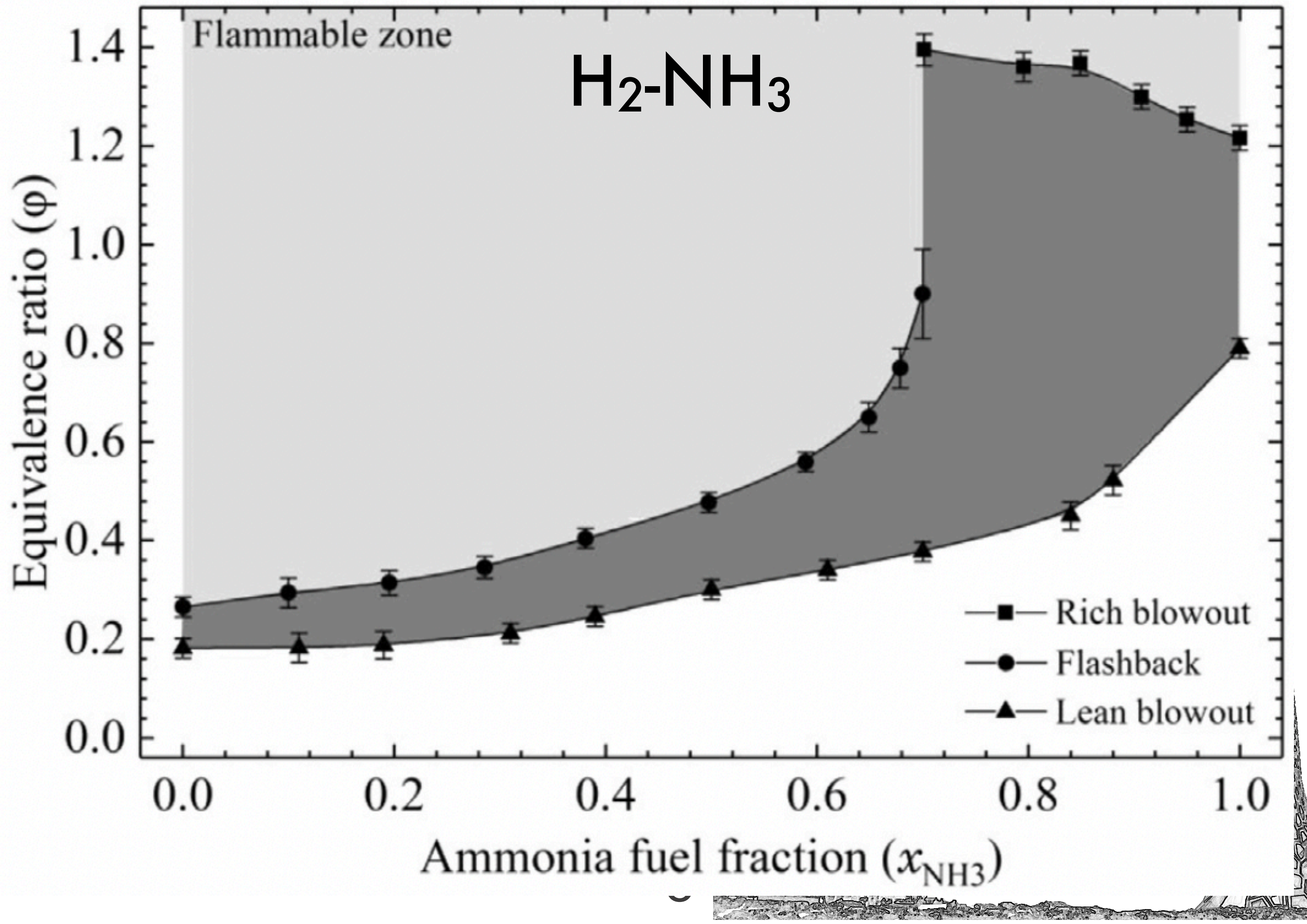
The dreaded flashback…

Because of their comparatively high turbulent flame speed and small quenching distance, H_2 flames are prone to flashback



Lab-scale swirl burner designed to withstand flashback

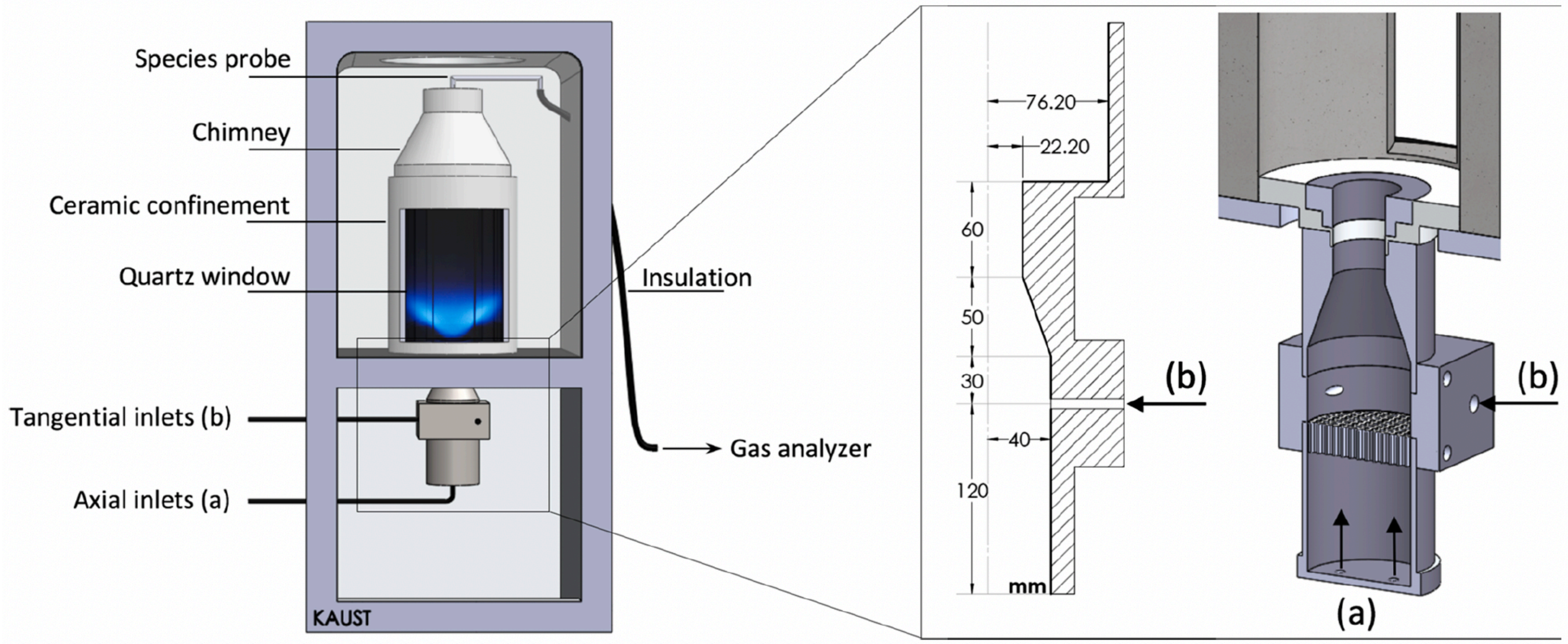




Khateeb et al. Exp. Therm. Fluid Sci. 2020(114)
Khateeb et al. Int. J. Hydrogen Energ. 2020(45)

The dreaded flashback…

Increasing pressure may promote flashback through effects of increasing turbulence intensity



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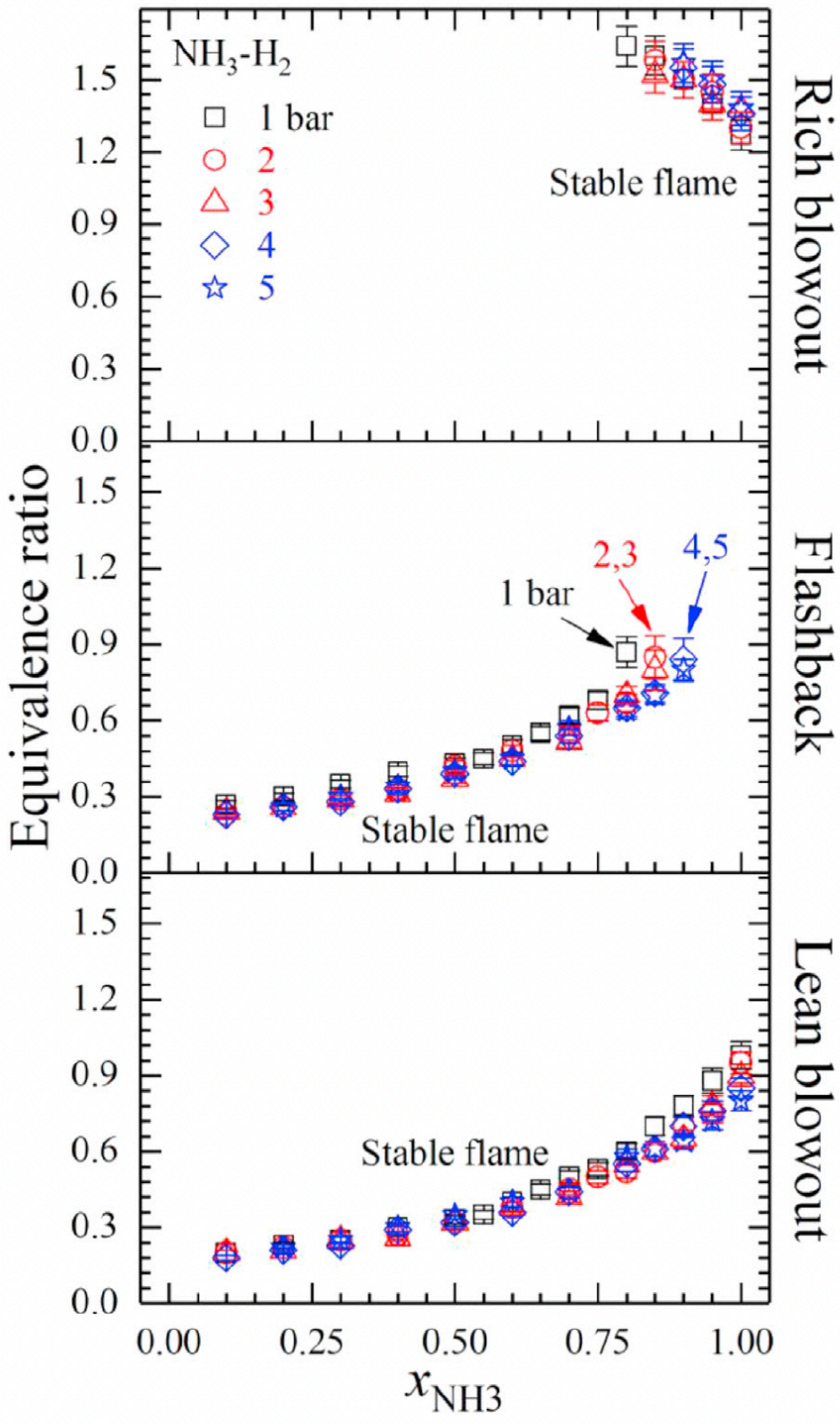
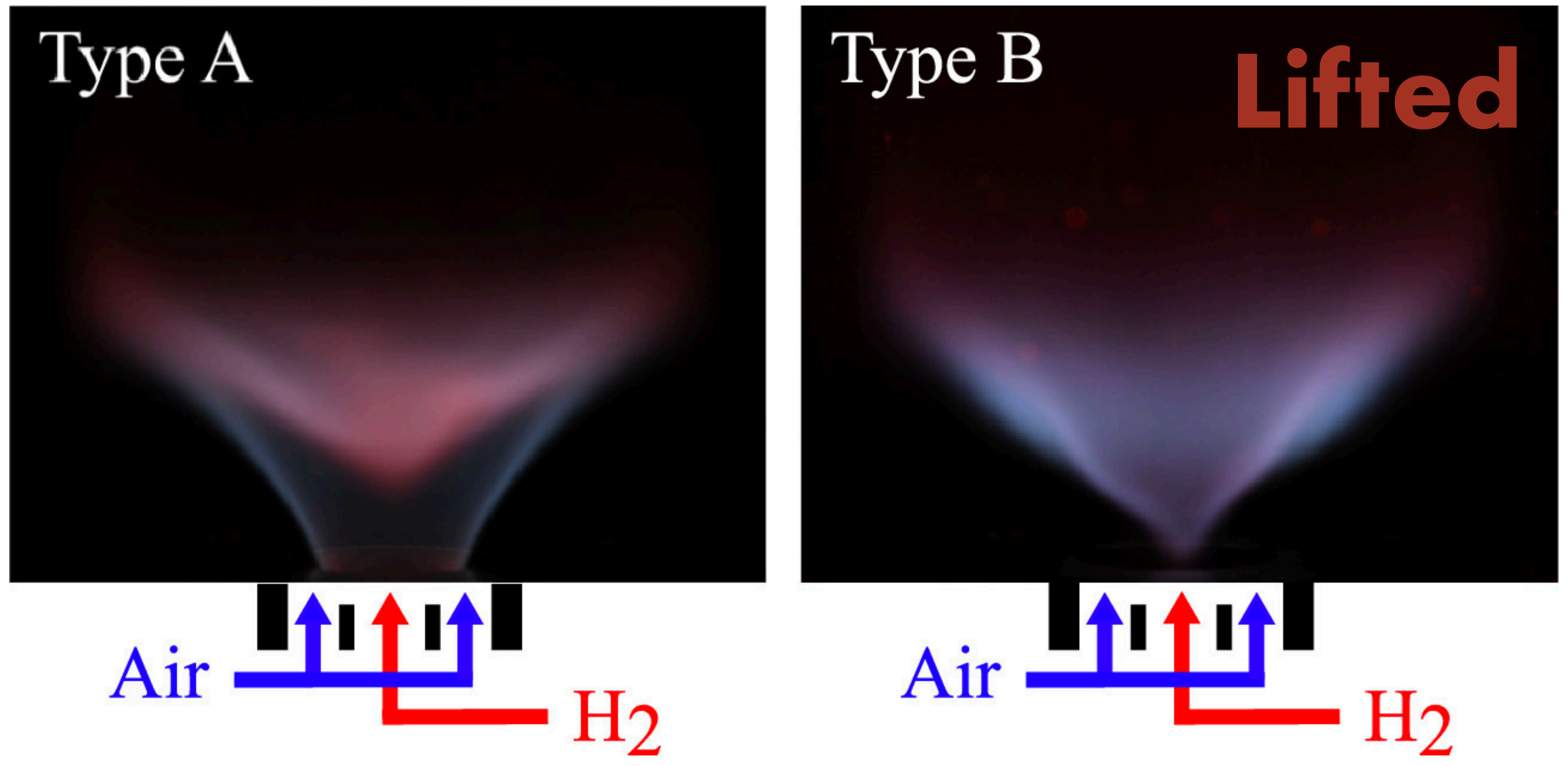


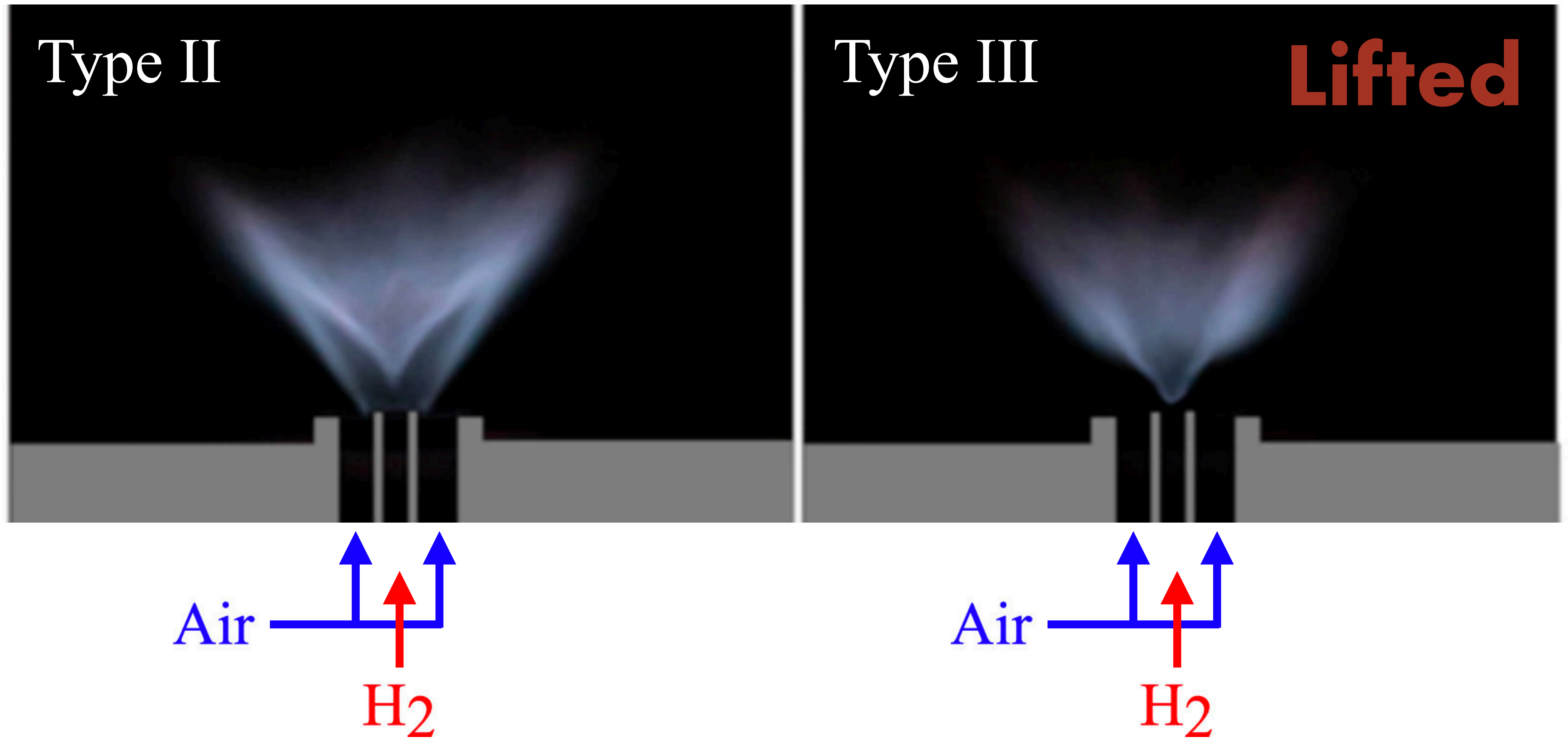
Khateeb et al. Int. J. Hydrogen Energ. 2021(46)

The convenience of dual swirl H_2-air flames

H_2-air flames stabilized with a dual swirl co-axial burner are promising candidates for the decarbonization of gas turbines



Marragou et al. Combust. Flame 2023
Marragou et al. Int. Proc. Combust. Inst. 2023
Marragou et al. Int. J. Hydrogen Energ. 2022



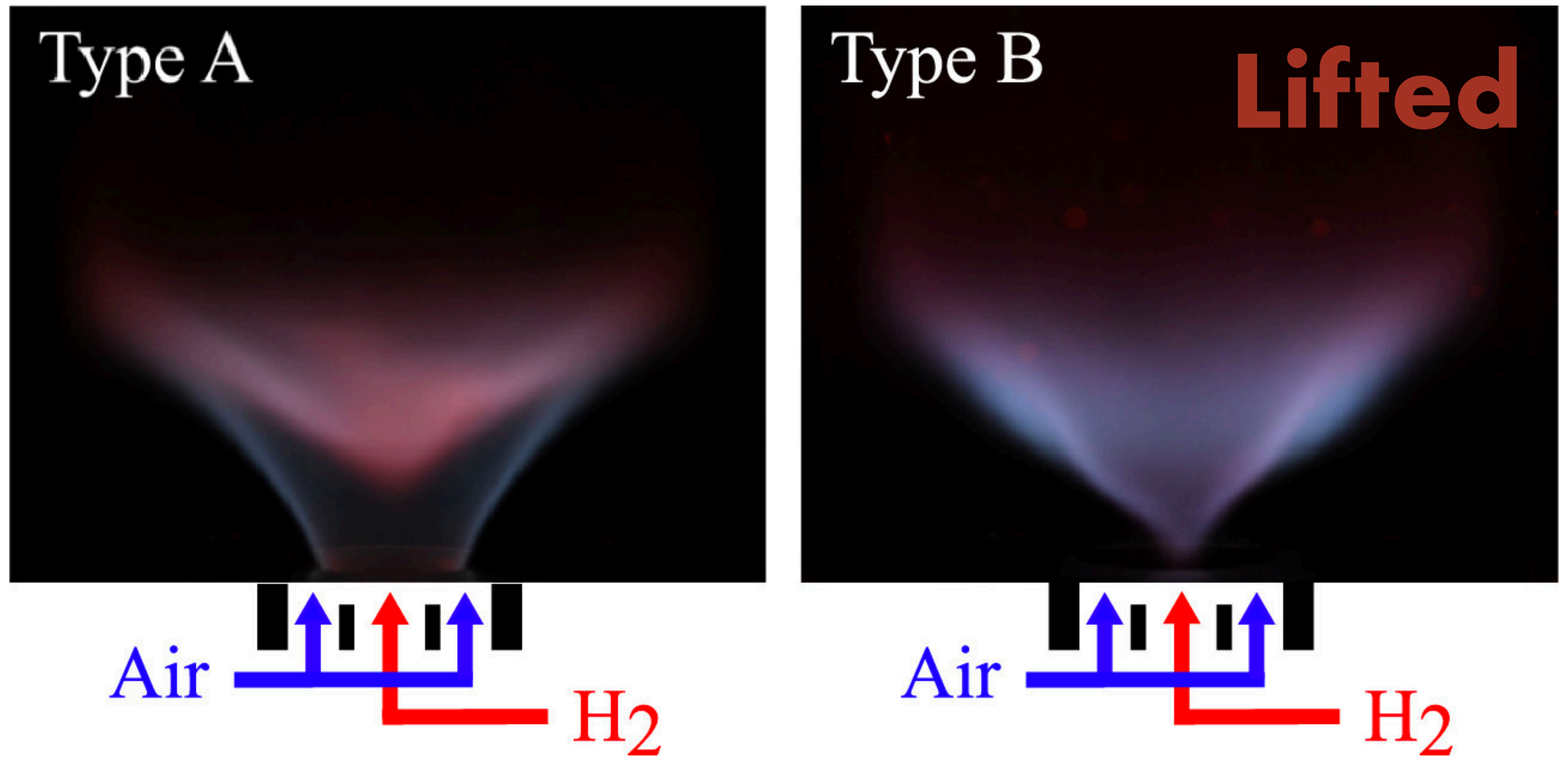
Leroy et al. J. Eng. Gas Turbines Power 2023

This technology is capable of achieving low NOx emissions while providing flashback protection and minimizing injector wall temperature

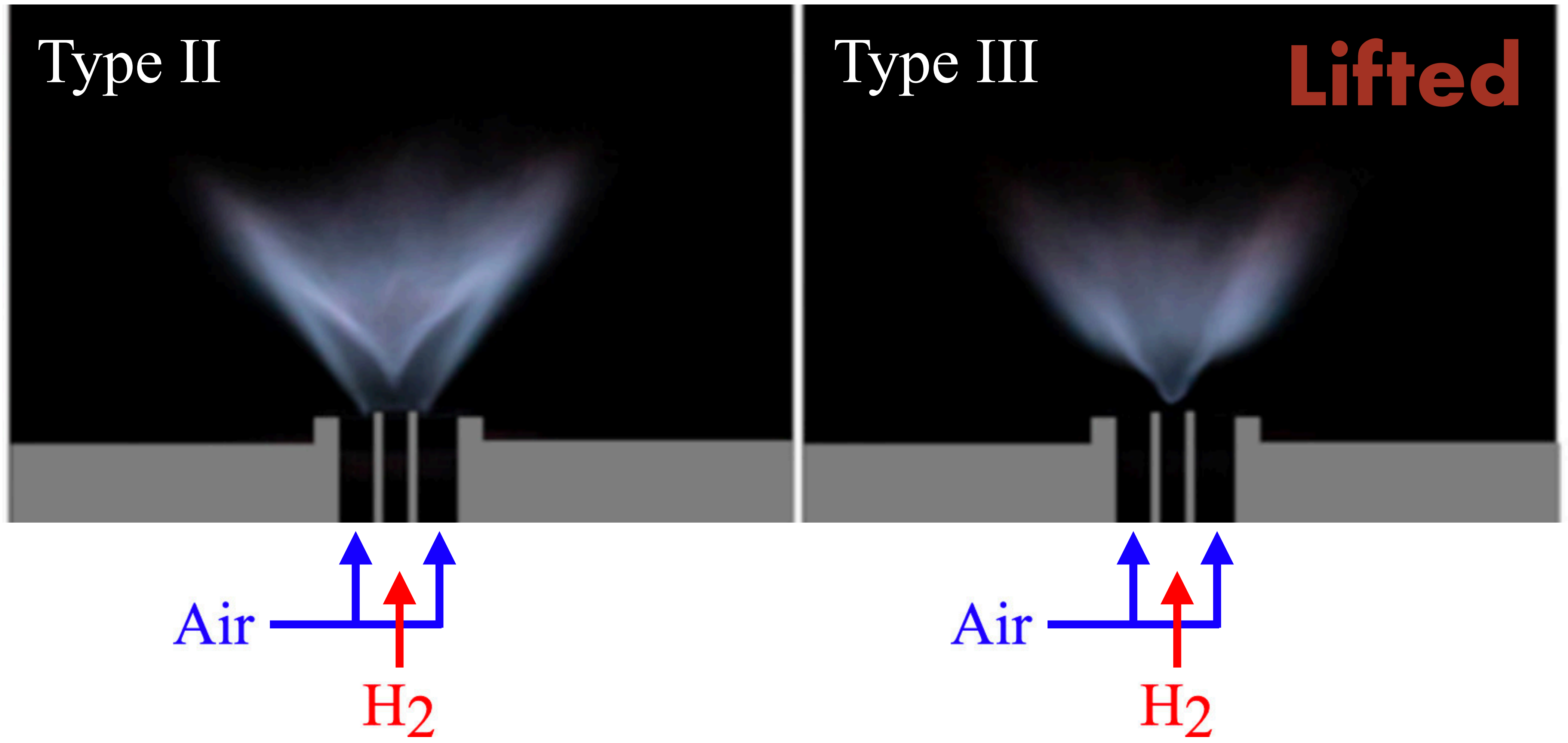
However, this implies maintaining the flame in the lifted regime

The convenience of dual swirl H_2-air flames

H_2-air flames stabilized with a dual swirl co-axial burner are promising candidates for the decarbonization of gas turbines



Marragou et al. Combust. Flame 2023
Marragou et al. Int. Proc. Combust. Inst. 2023
Marragou et al. Int. J. Hydrogen Energ. 2022



Leroy et al. J. Eng. Gas Turbines Power 2023

There is a need to understand the physical mechanism(s) leading to the detachment and reattachment of these flames

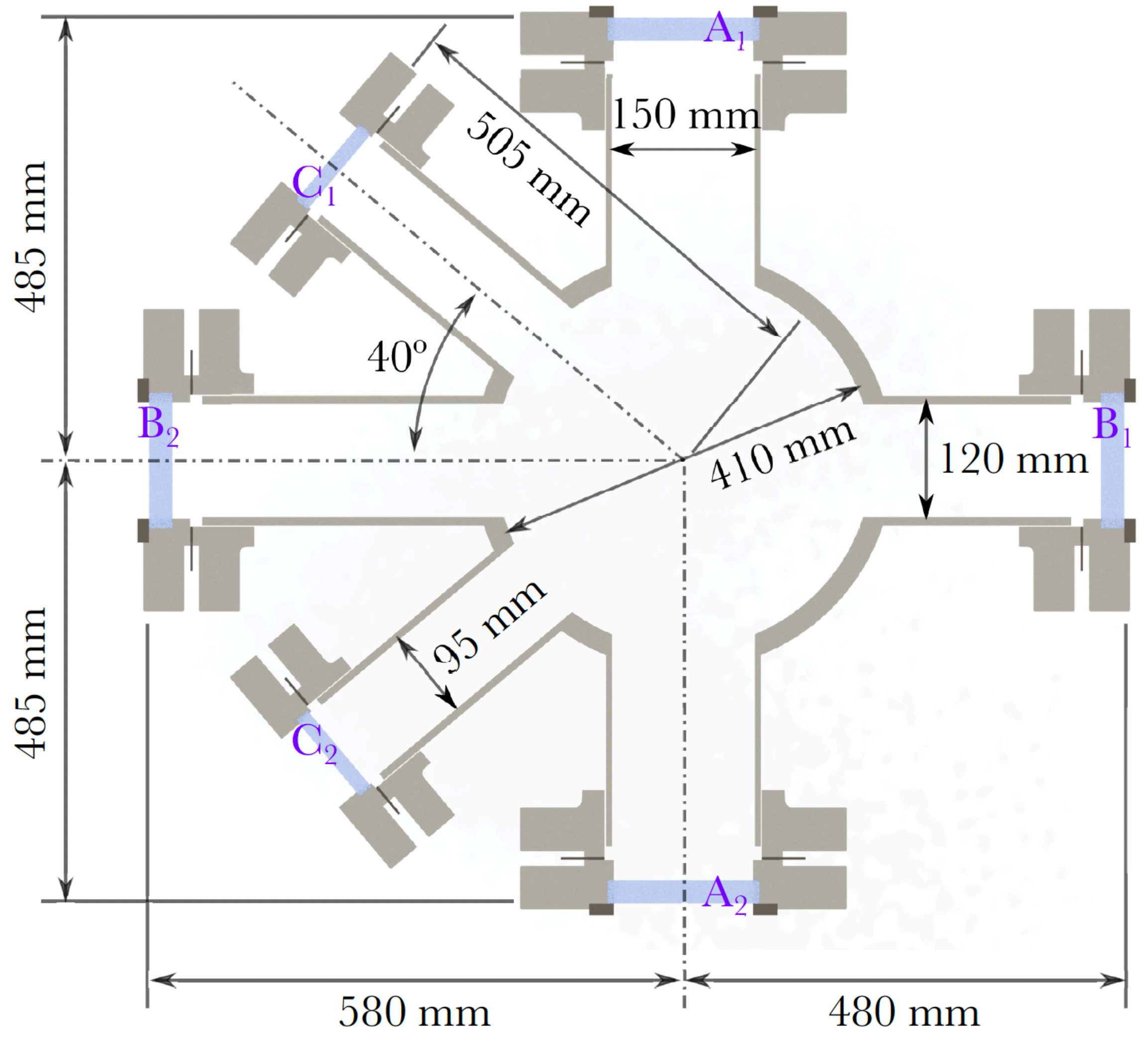
With practical applications in mind, effects of elevating pressure must be understood too

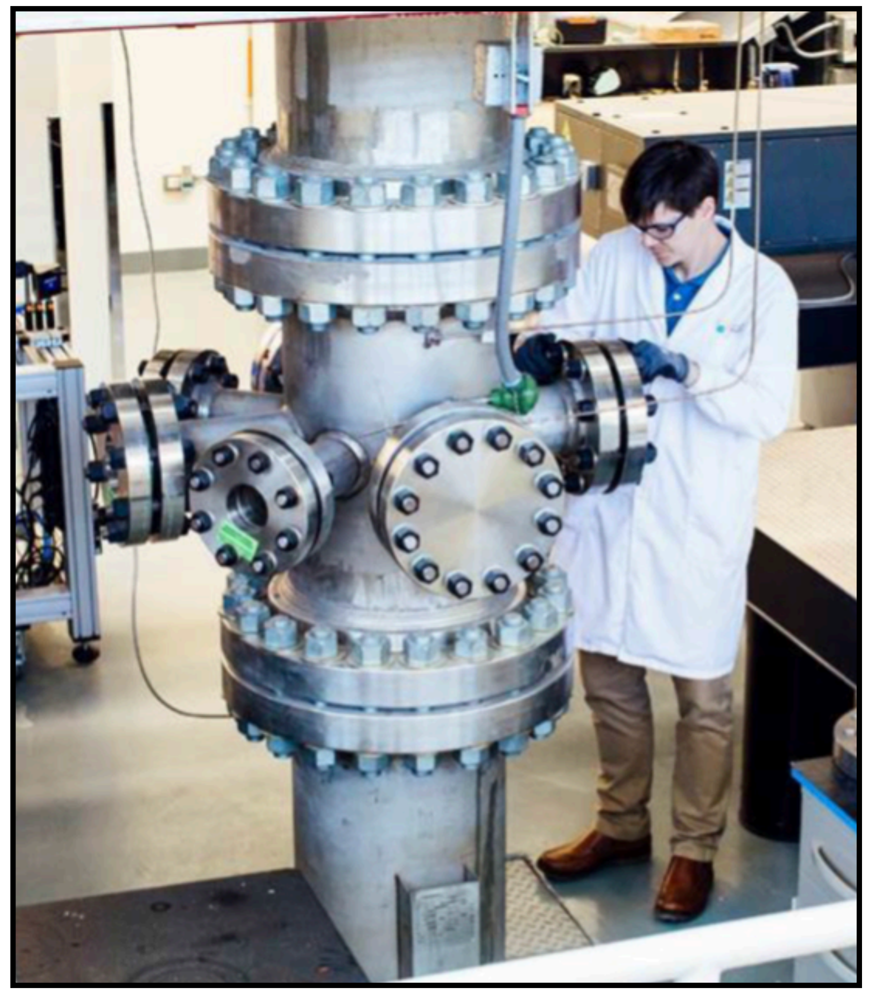
KAUST's High Pressure Combustion Duct (HPCD)

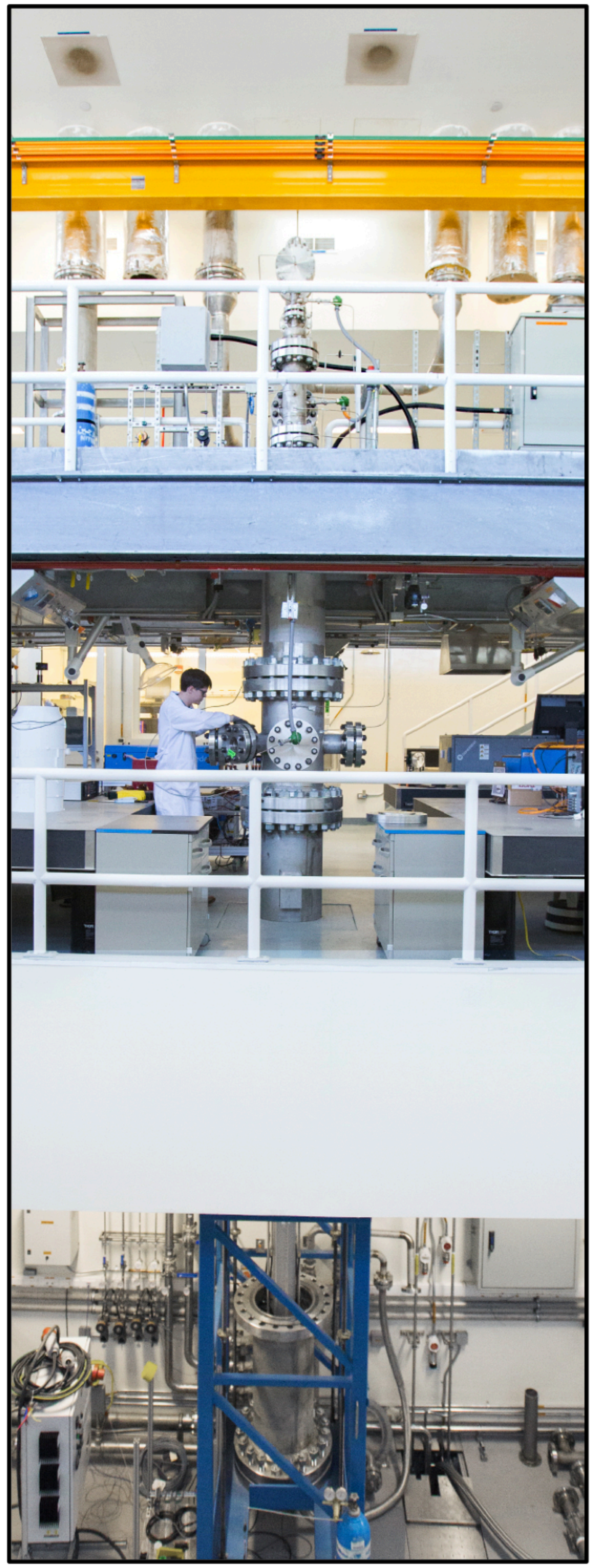
The HPCD is one of the high-pressure test-rigs available at CCRC in KAUST

9-m tall & vertical

40 bar
>100 kW @ steady state



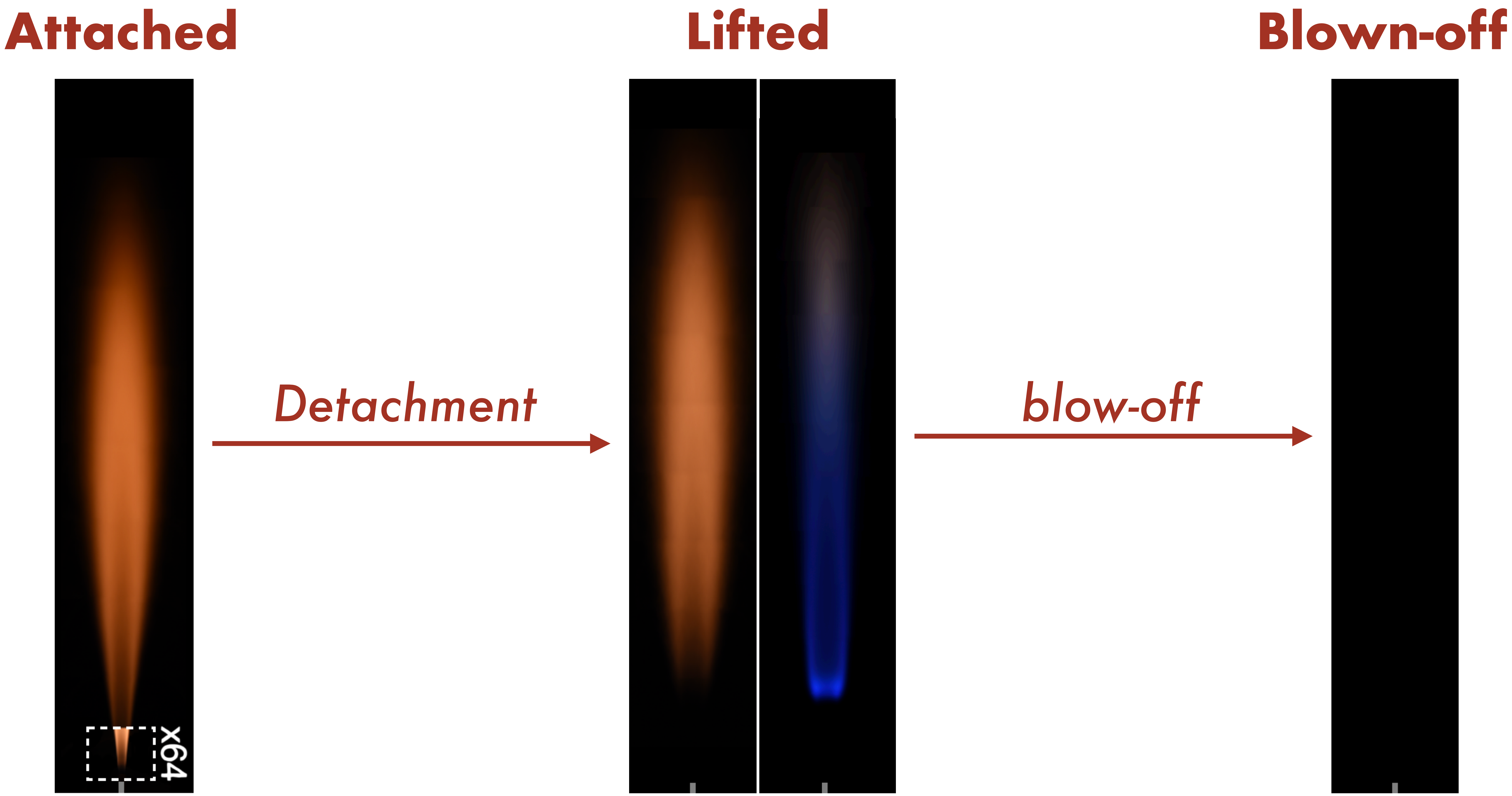




Ample optical access

Turbulent non-premixed jet flames

Turbulent non-premixed jet flames can be found in three states:



Can we predict these transitions for any fuel, pressure, nozzle geometry?

This is important for flares, punctured fuel tanks, furnaces, etc… **and H_2 swirl flames**

Flame detachment

From previous work at 1 bar (e.g. Takahashi and Schmoll, Proc. Combust. Inst., 1991), two detachment mechanisms are typically observed:

δ decreases with P!

$\delta >> t$

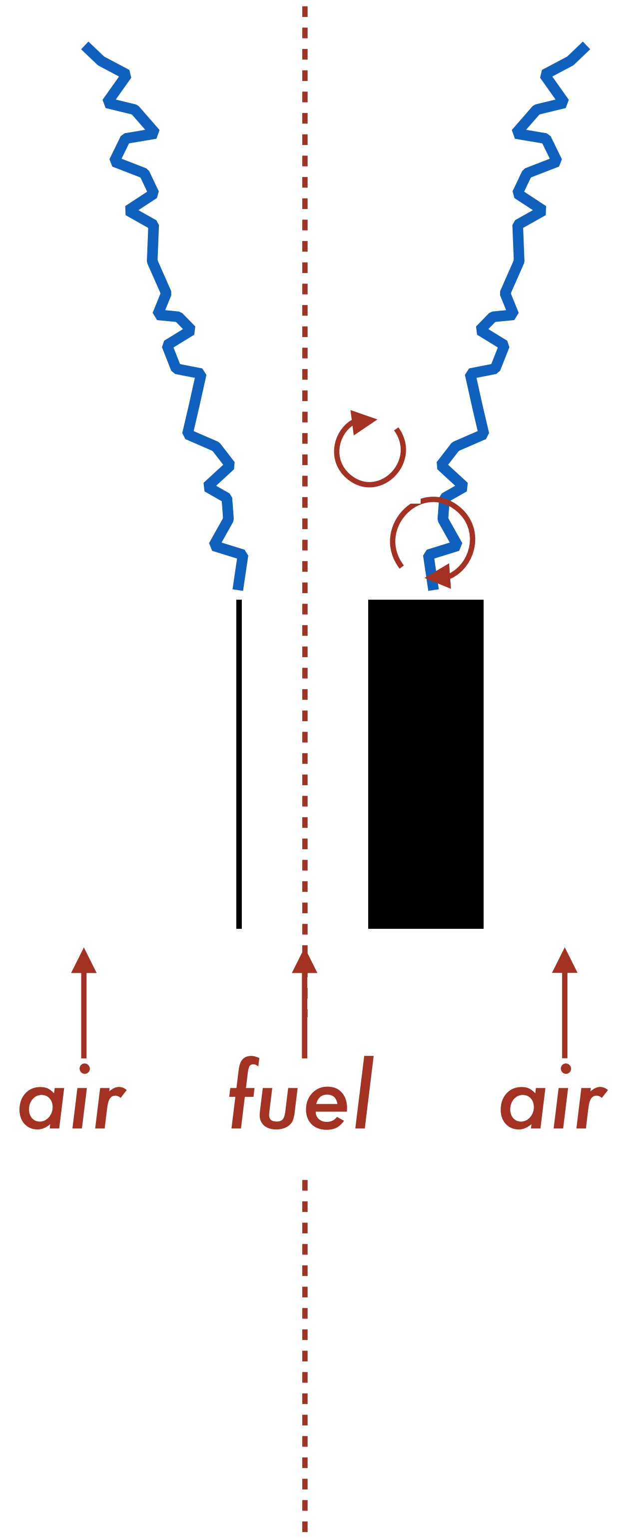
If the flame thickness δ is larger than the rim thickness t:

↓

The flame edge is exposed to the incoming flow

↓

Aerodynamic detachment



$\delta << t$

If the flame thickness δ is smaller than the rim thickness t:

↓

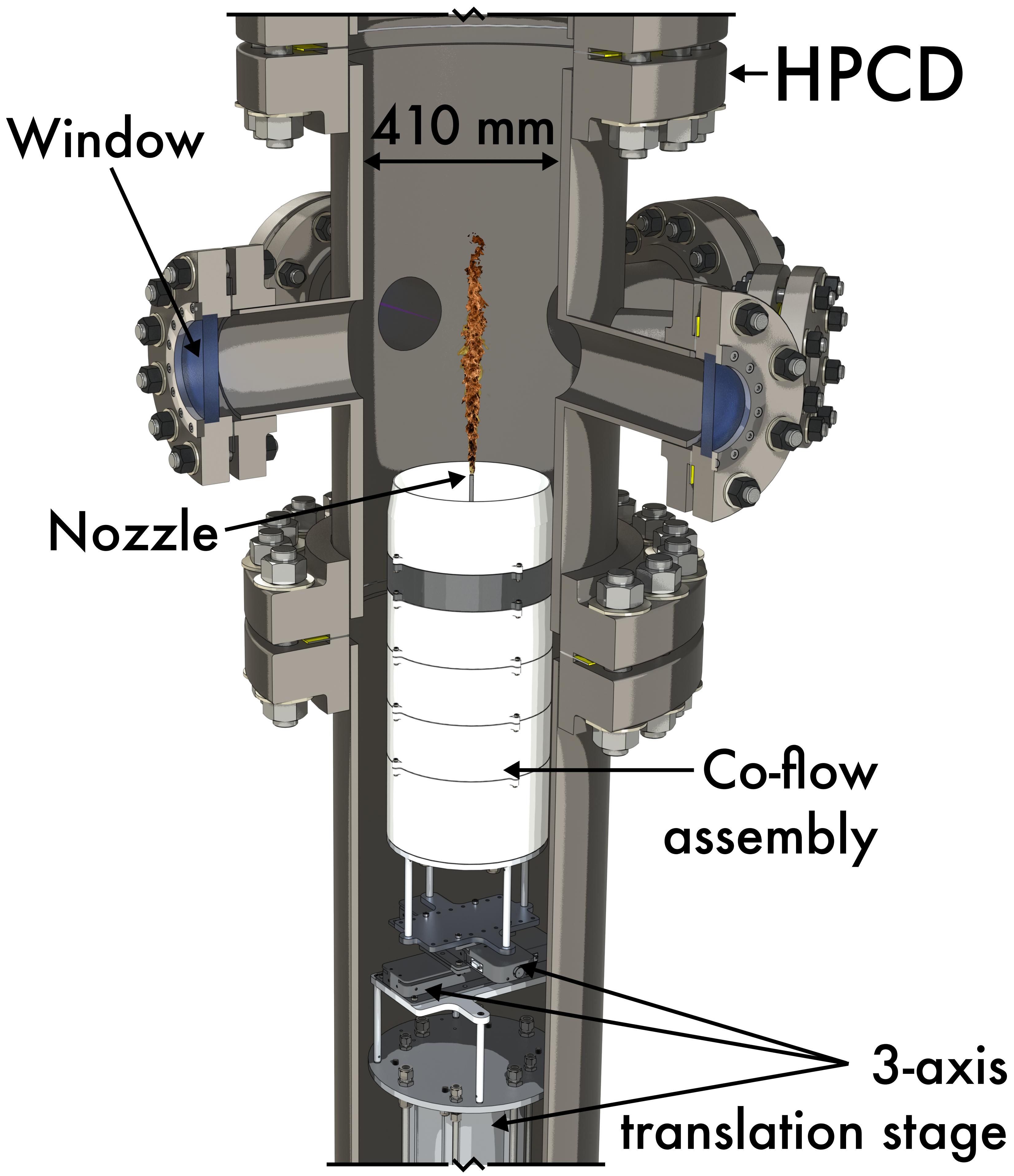
The flame edge is protected from the incoming flow

↓

Detachment by turbulence-induced local extinction

Can we predict detachment quantitatively? *i.e.*, can we model detachment $U_d = f(x,y,...)$?

Flame detachment



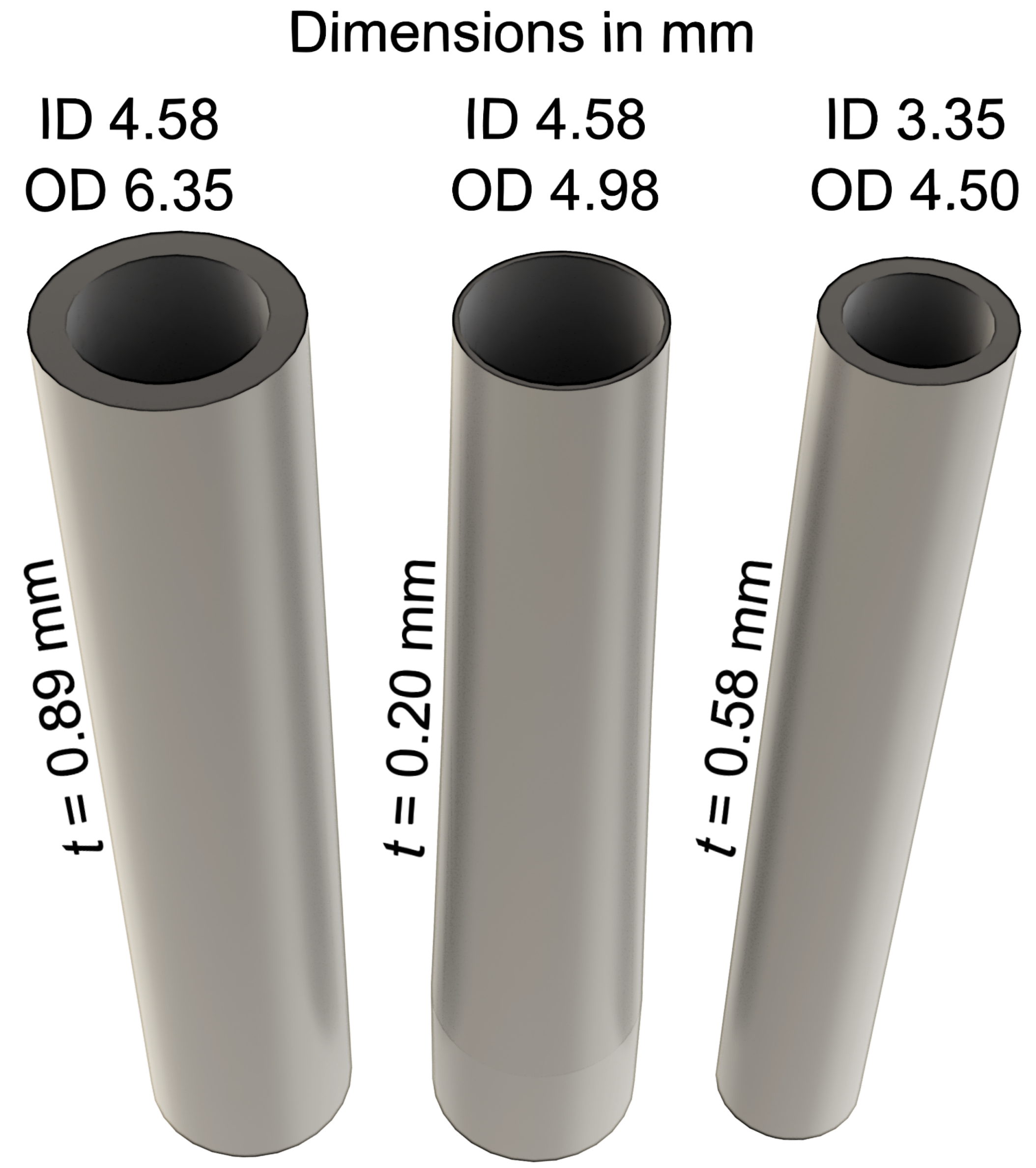
Fuels: methane & ethane

Pressures: $1 \leq P \leq 10$ bar

Jet velocities: $0.5 \leq U_j \leq 25$ m/s

Co-flow velocities: $0.3 \leq U_c \leq 0.9$ m/s

Reynolds numbers: up to 48,000

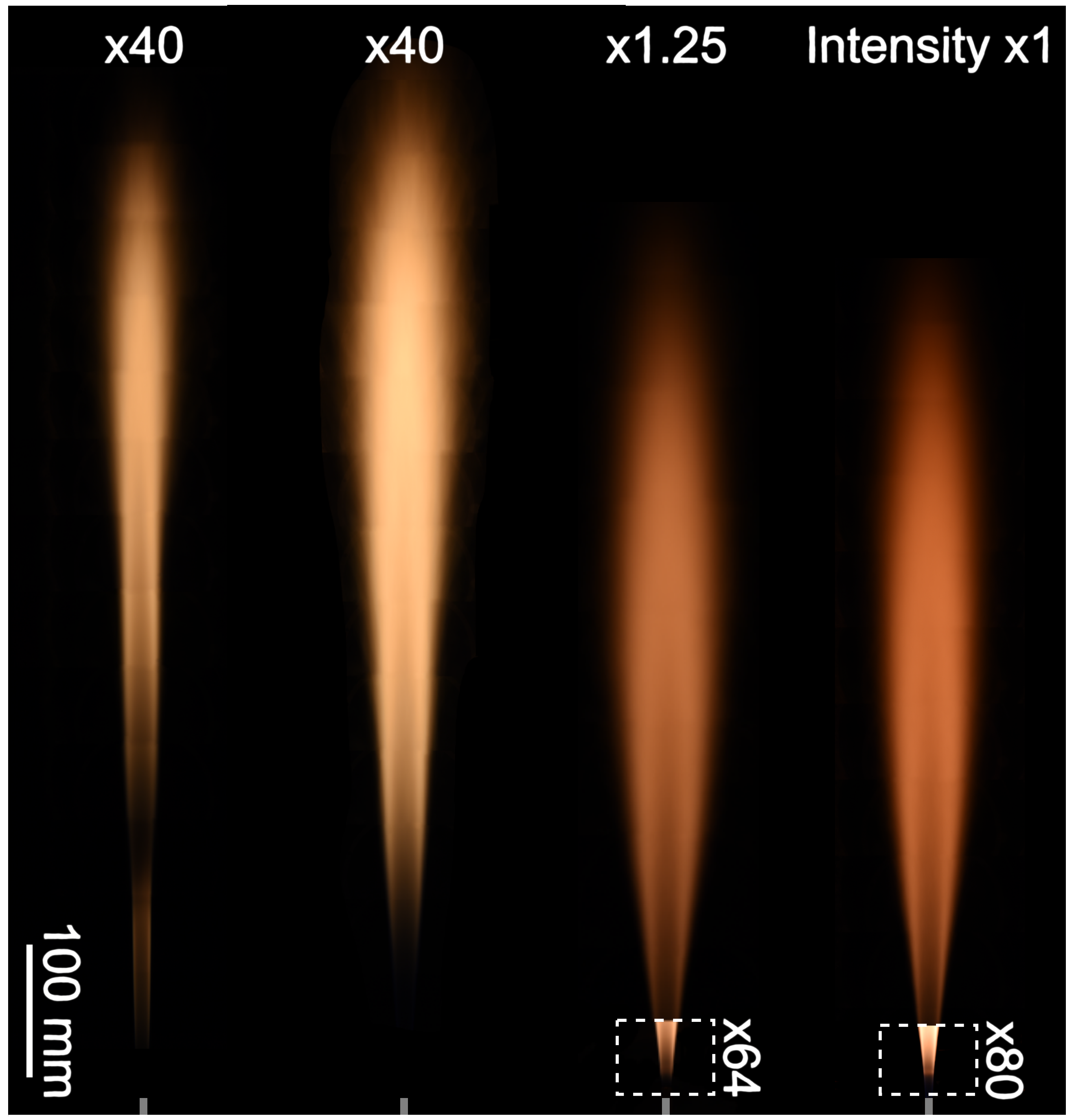


Instantaneous shots, stitched DSLR (6 bar)

Flame detachment

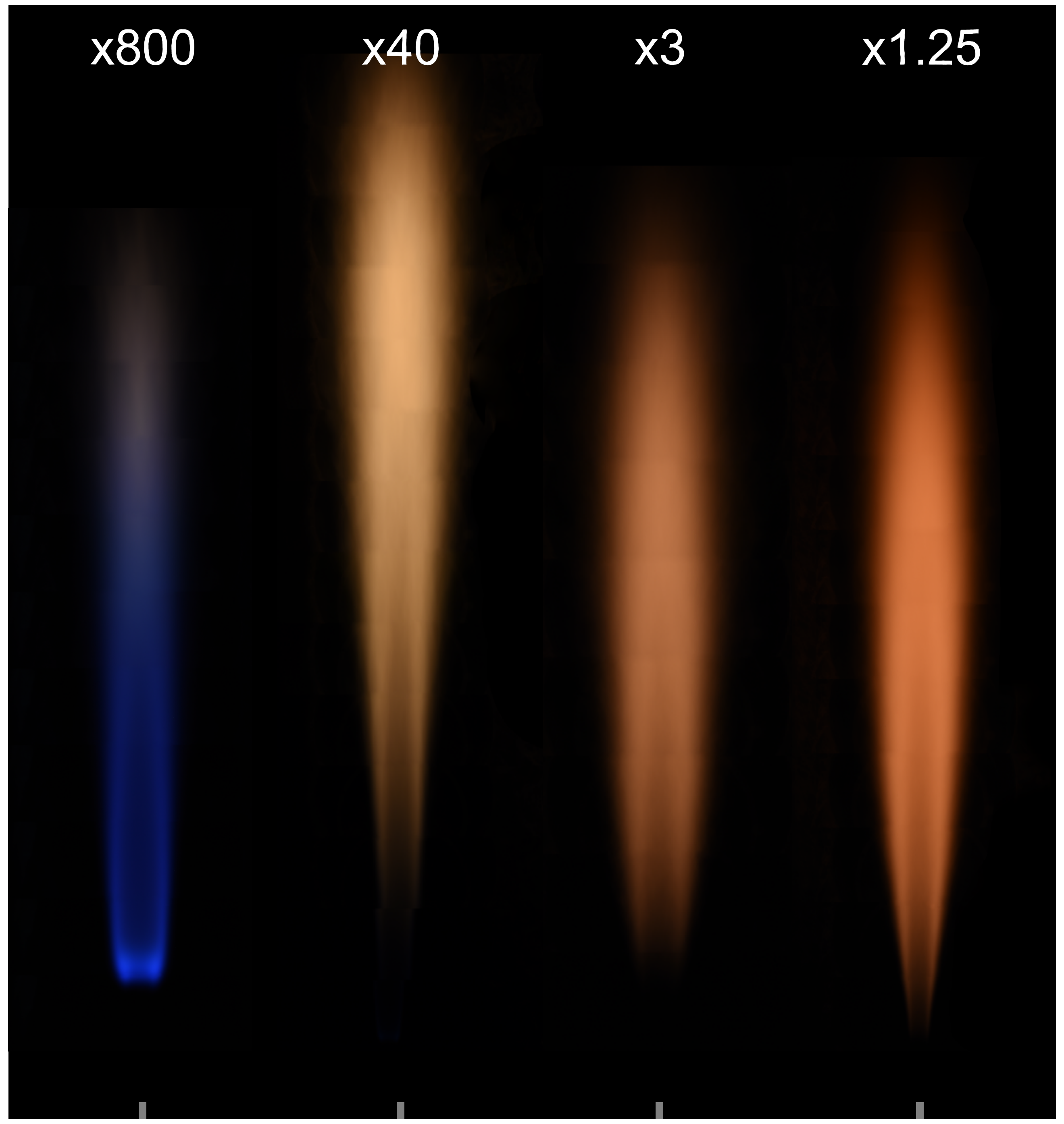
Attached

Methane	Ethane	Methane	Ethane
1 bar	1 bar	10 bar	6 bar
U_j = 12 m.s^{-1}	10	7	10
U_c = 0.6 m.s^{-1}	0.6	0.3	0.6
Re = 2397	5062	13985	30373



Lifted

Methane	Ethane	Methane	Ethane
1 bar	1 bar	7 bar	6 bar
U_j = 24 m.s^{-1}	15	10	13
U_c = 0.6 m.s^{-1}	0.6	0.3	0.6
Re = 4795	7593	13985	39485

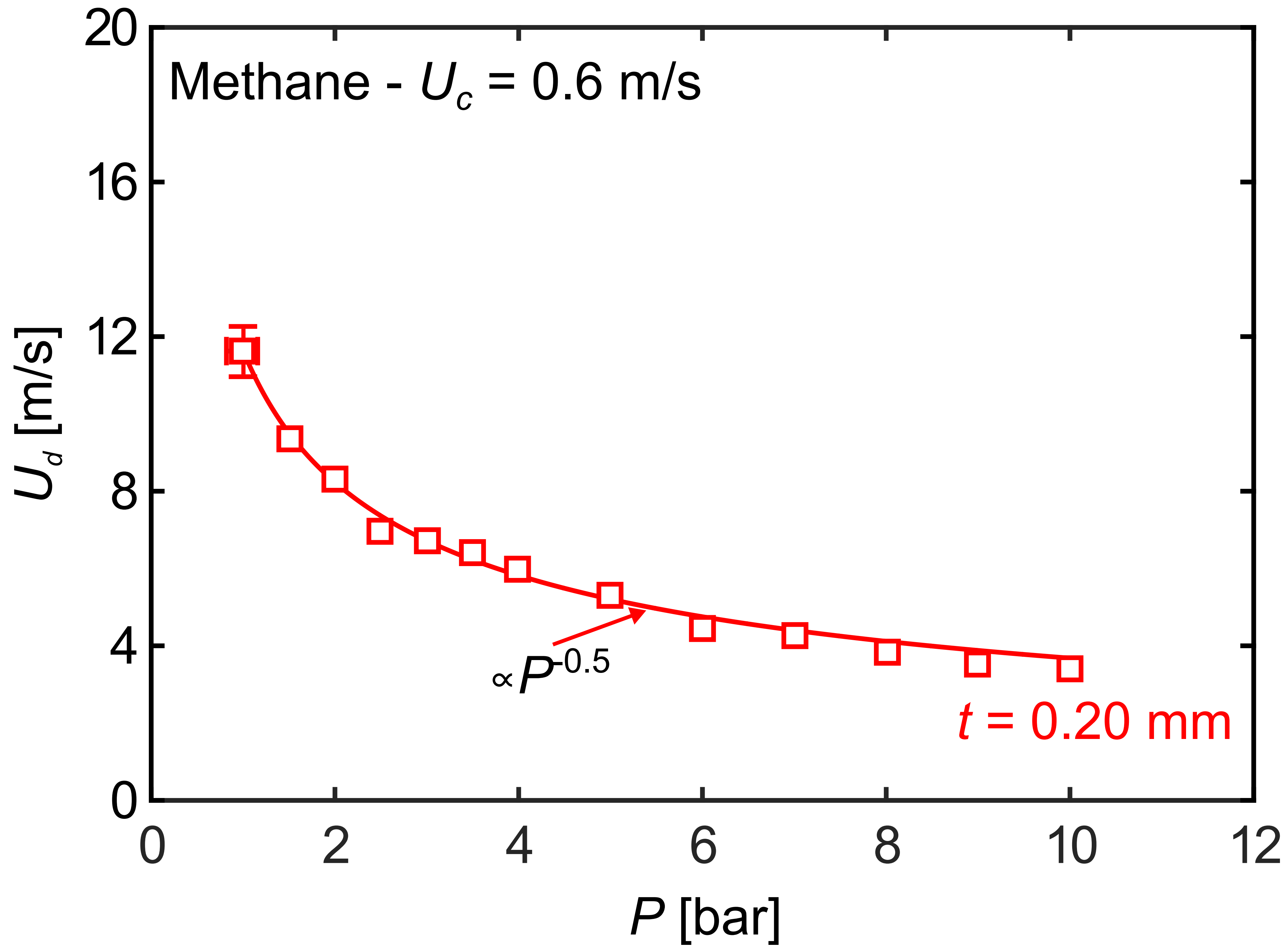


Starting with an attached flame, the jet velocity was increased progressively until detachment occurs. Detachment events were detected by eye

Guiberti et al. Combust. Flame 2019(203)

Flame detachment

Effect of pressure



If t = 0.20 mm, U_d decreases monotonically with P
It scales with $P^{-0.5}$

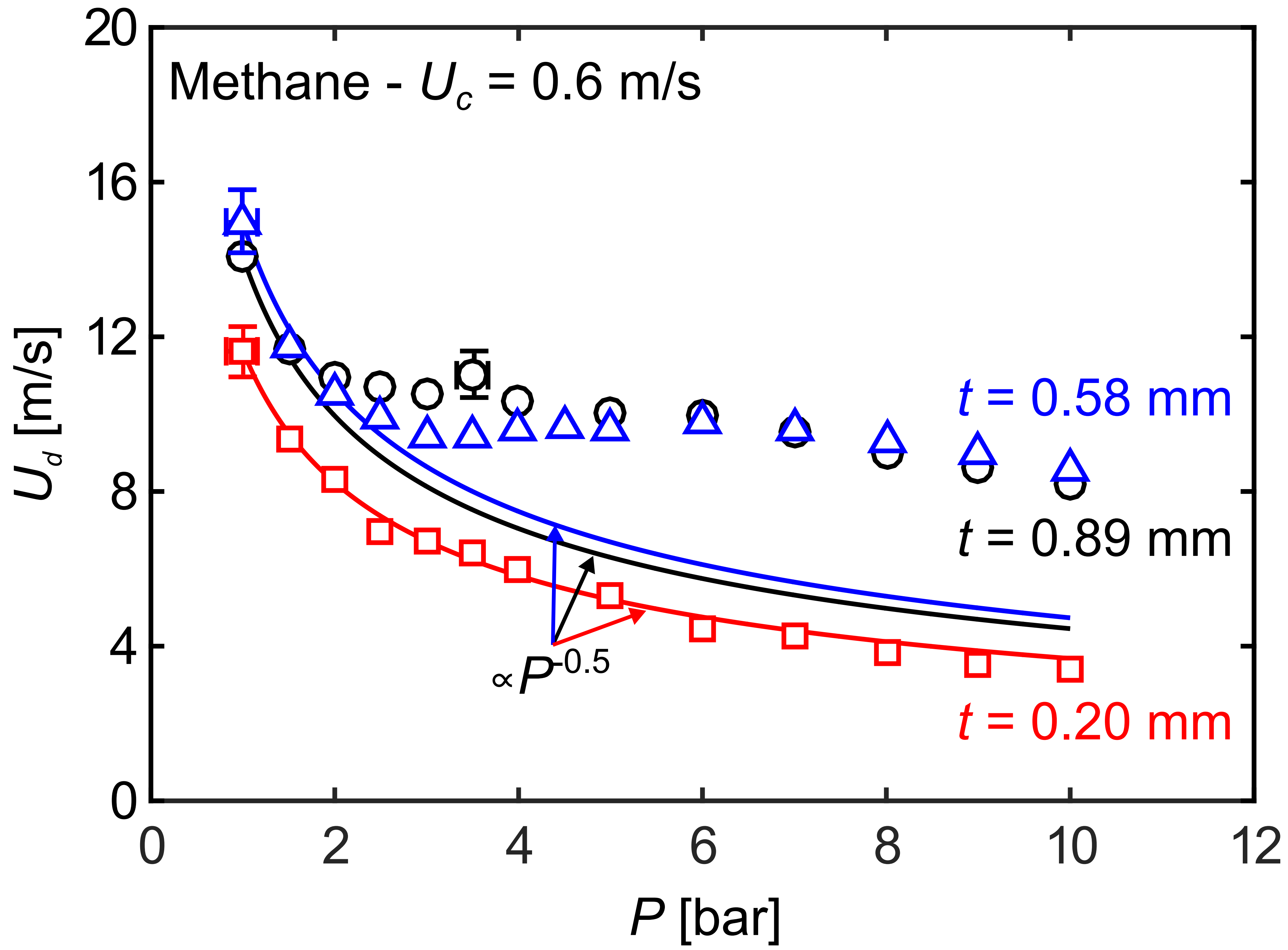
For methane, the laminar burning velocity S_L also scales with $P^{-0.5}$

➡ If t = 0.20 mm, U_d and S_L are proportional

These experimental observations are consistent with aerodynamic detachment

Flame detachment

Effect of the nozzle thickness



Regardless of t, there is a critical P below which U_d scales with $P^{-0.5}$

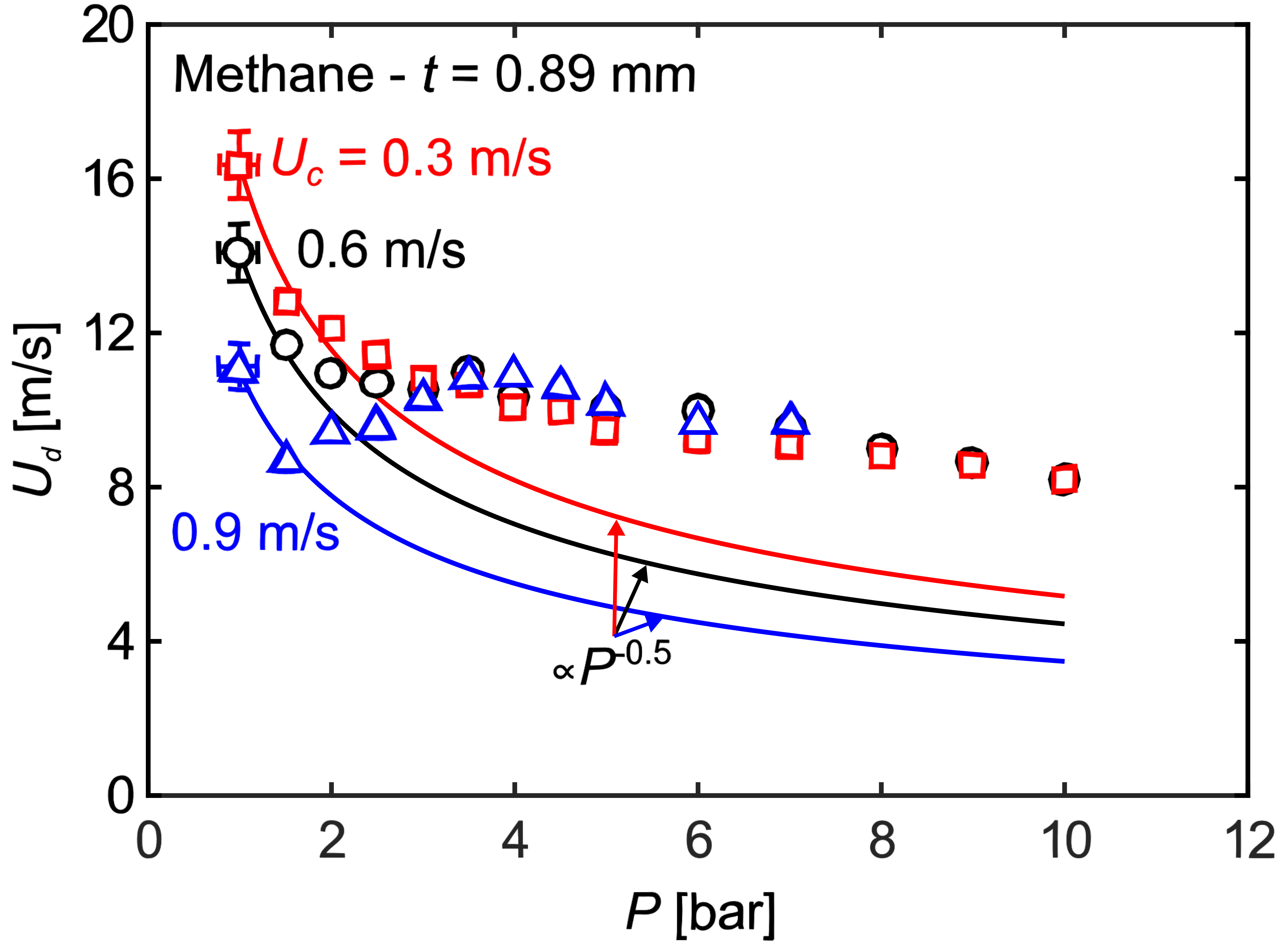
If t = 0.58 or 0.89 mm, a non-monotonic behavior is observed

➡ This suggests that the detachment mechanism changes as pressure increases

 Guiberti et al. Combust. Flame 2019(203)

Flame detachment

Effect of the co-flow



If t = 0.89 mm and P < 3 bar, U_d is a function of U_c

➡ Aerodynamic detachment

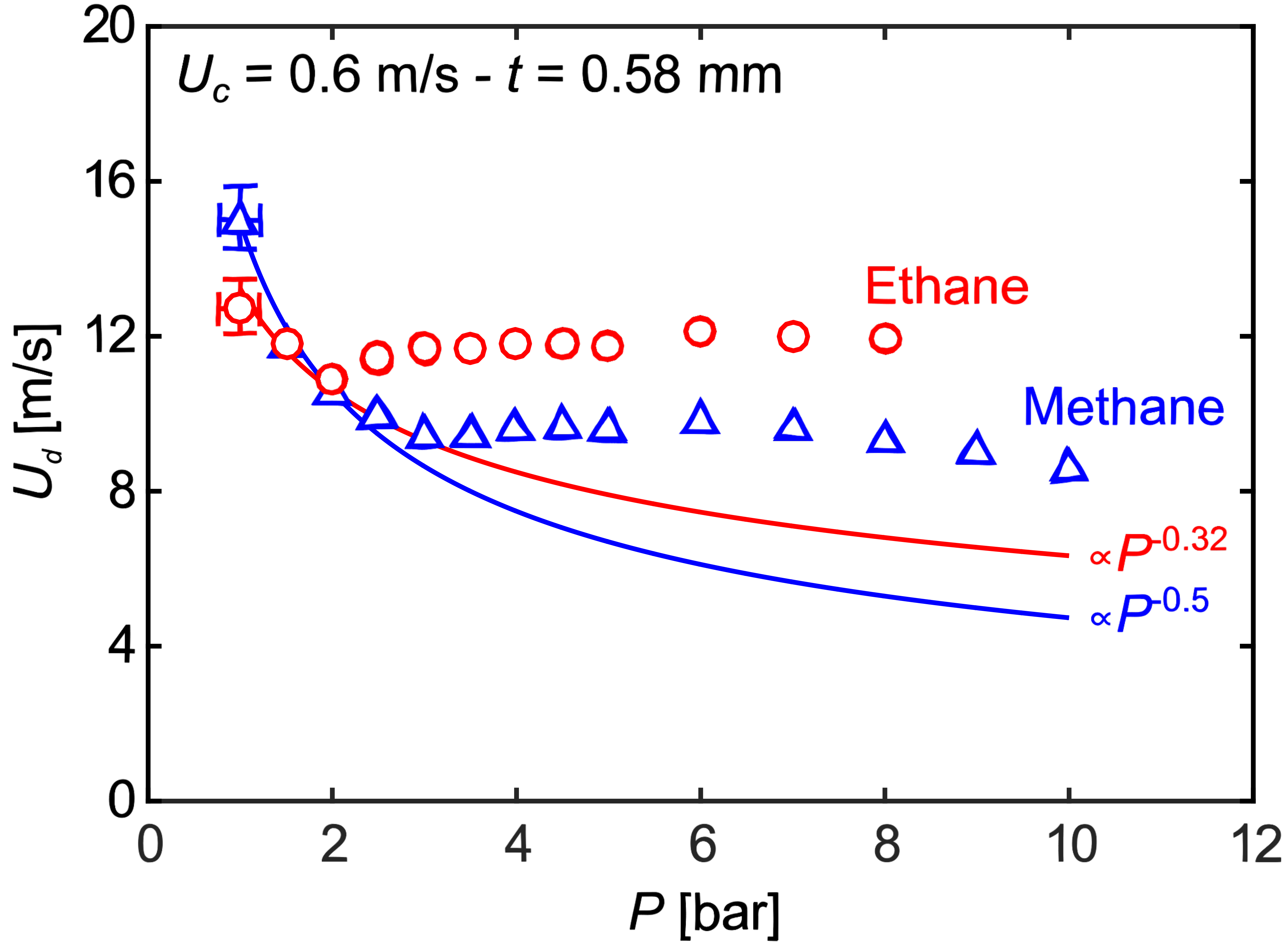
If t = 0.89 mm and P > 3 bar, U_d is not a function of U_c

➡ Detachment by local extinction?

Guiberti et al. Combust. Flame 2019(203)

Flame detachment

Effect of the fuel



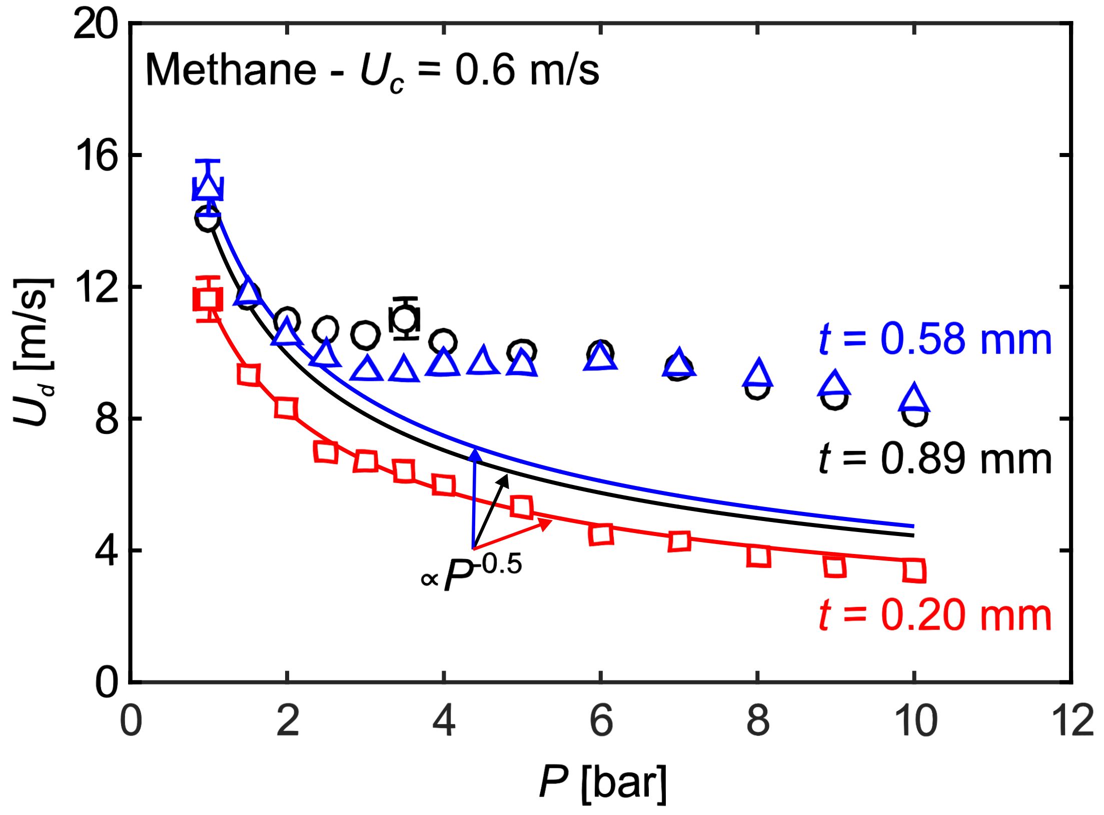
For ethane, if $P < 2$ bar, U_d is also proportional to S_L for ethane because S_L scales with $P^{-0.32}$

If $P > 2$ bar, ethane jet flames are more resistant to detachment

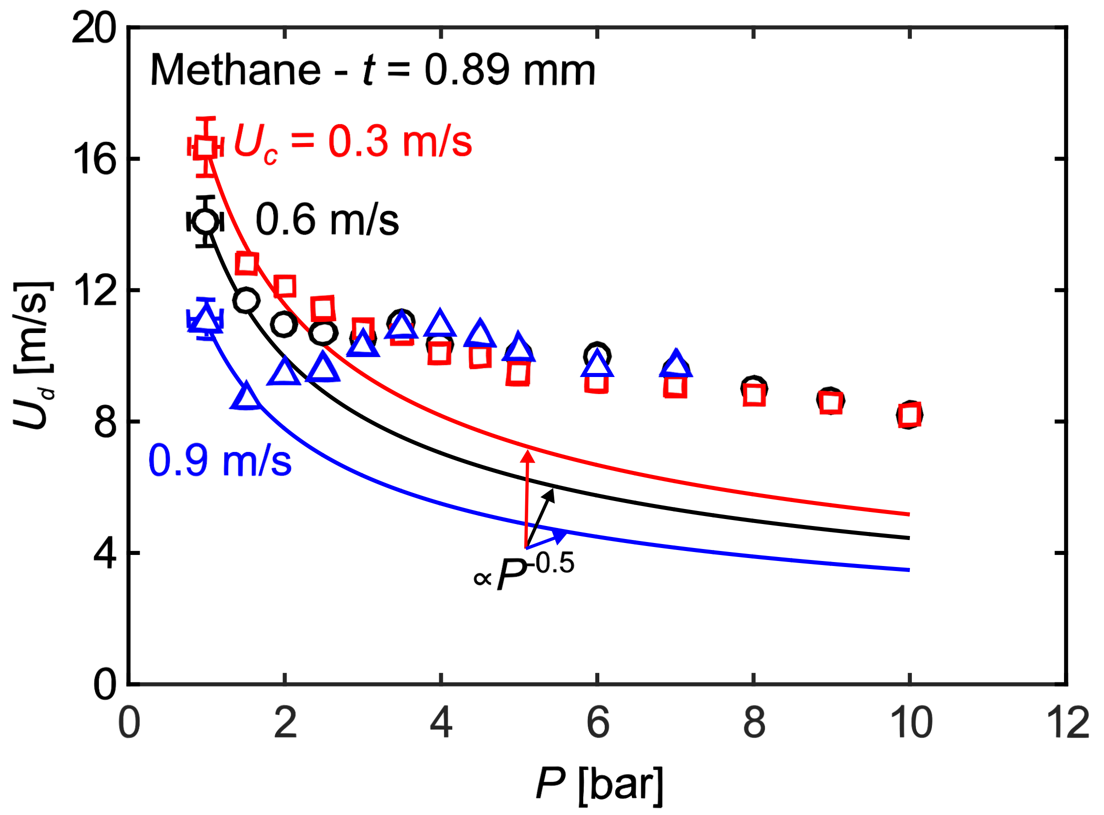
Guiberti et al. Combust. Flame 2019(203)

Flame detachment

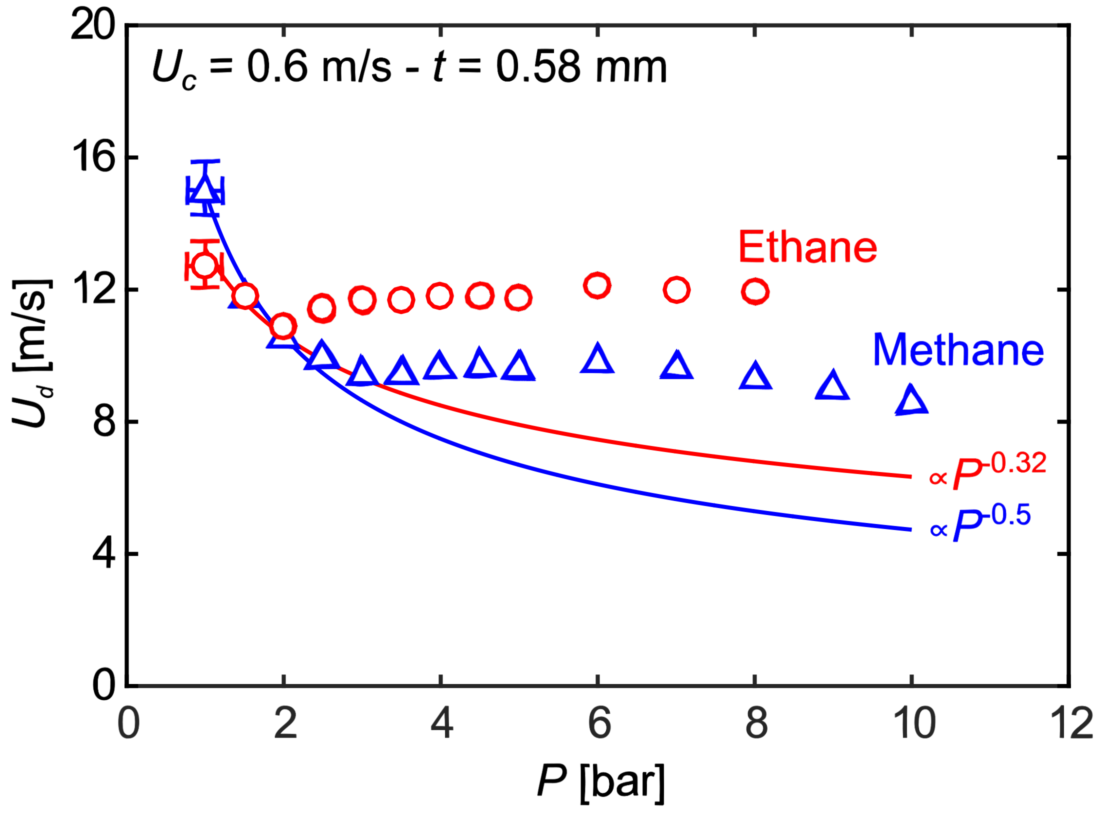
Pressure & thickness



Co-flow



Fuel



Increasing pressure allows to continuously cross boundaries between detachment mechanisms

➡ This is useful to develop models and predictive tools

This is "*harder*" to achieve with fuel or nozzle thickness

Effects of the mixture fraction

Boring to test > 10 nozzles

Guiberti et al. Combust. Flame 2019(203)

Flame detachment

$t < 3\delta$

↓

Aerodynamic detachment

↓

$$U_d = S_L/U_c \times f(\xi_{st})$$

ξ mixture fraction

The detachment velocity can be predicted for any fuel and pressure as long as it is known at one pressure and $t < 3\delta$

$t = 3\delta$

$t > 3\delta$

↓

U_d does not depend on t and U_c

↓

But U_d cannot be predicted yet…

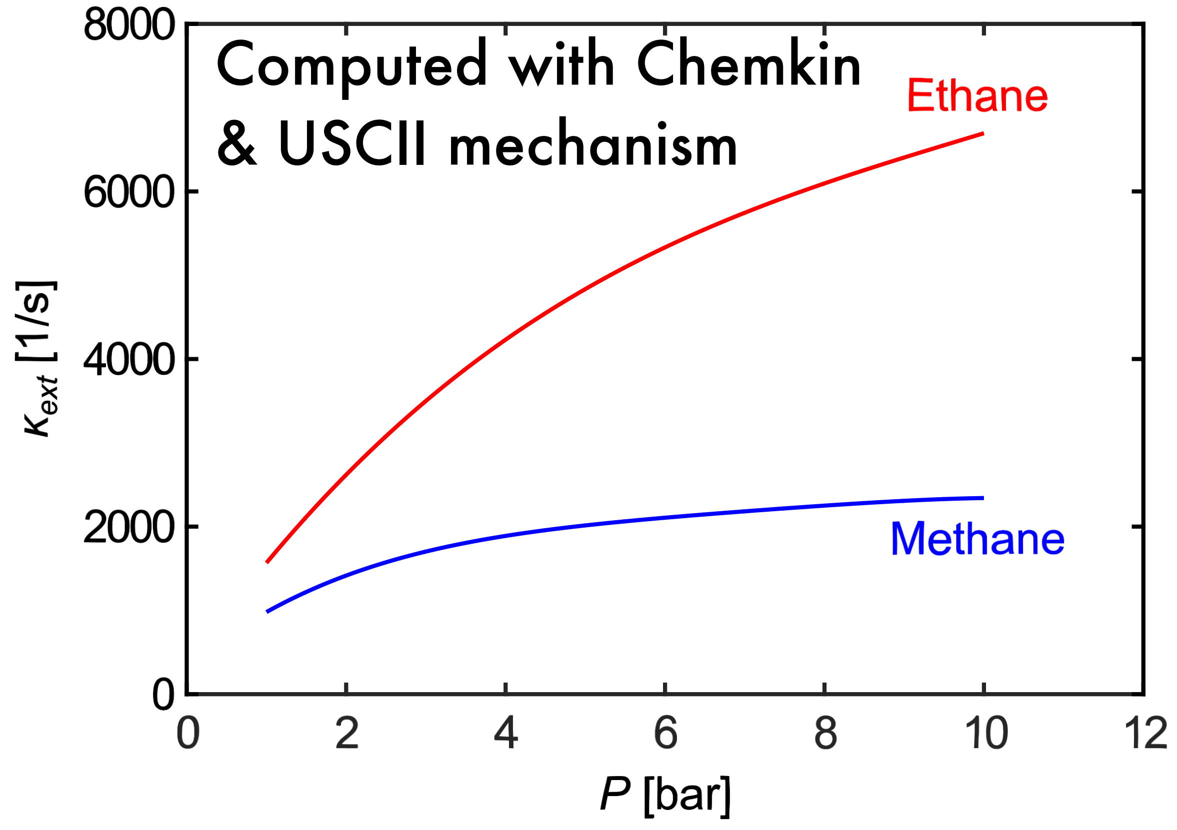
From previous work at 1 bar, detachment is triggered by localized flame extinction

Guiberti et al. Combust. Flame 2019(203)

Flame detachment

Extinction of a flame front occurs when the flow time scale τ_f becomes smaller than the chemical time scale τ_c

The chemical time scale τ_c can be approximated here as the inverse of the extinction strain rate



For non-premixed flames, the flow time scale controlling local extinction is the fastest, *i.e.*, the Kolmogorov time scale of turbulence τ_η

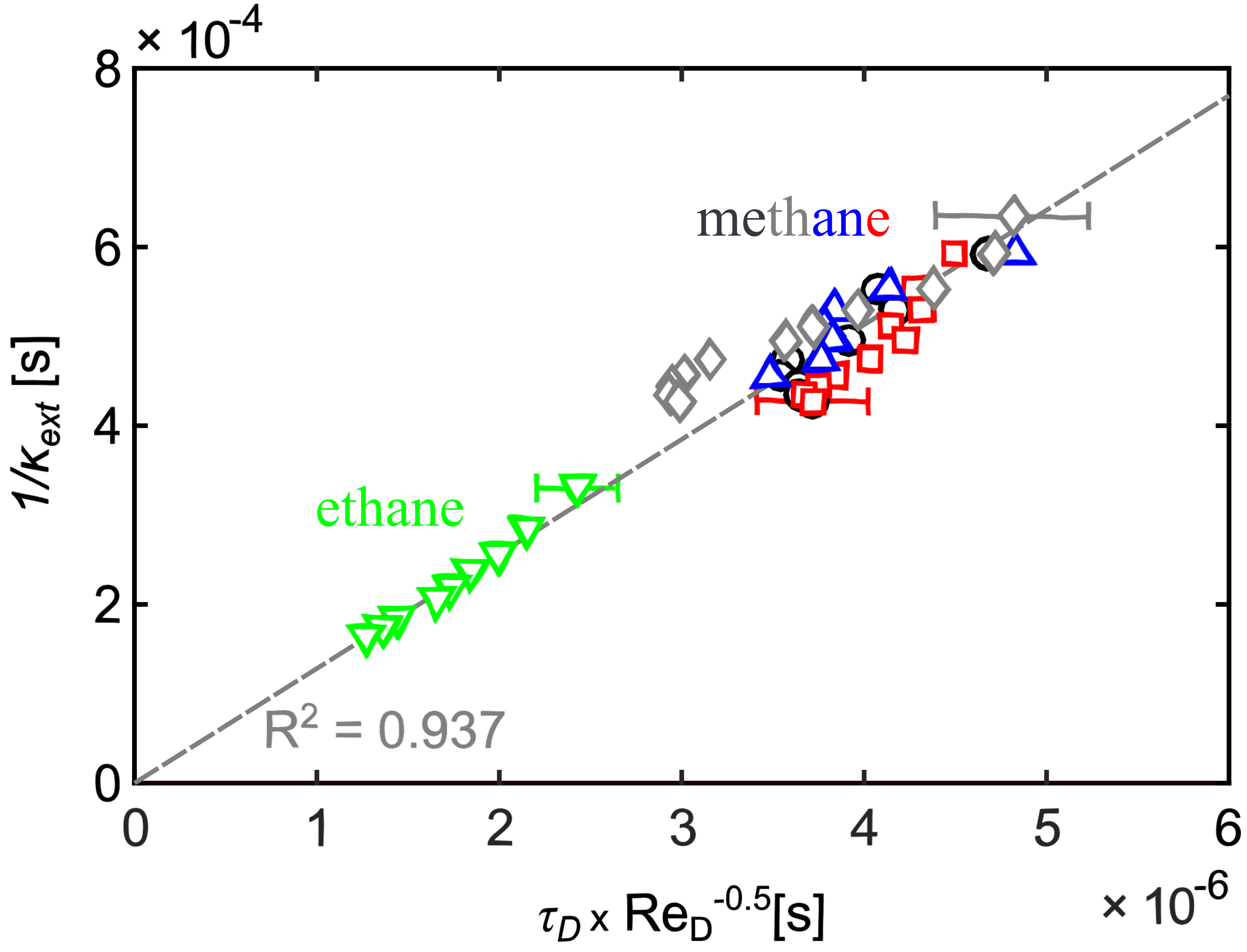
$$\tau_\eta \propto \tau_D \mathrm{Re}_D^{-0.5}$$

$$\tau_D = \frac{D}{U_j} \qquad \mathrm{Re}_D = \frac{U_j D}{\nu}$$

assumes homogeneous isotropic turbulence

Guiberti et al. Combust. Flame 2019(203)

Flame detachment



$$U_D = 128 D \mathrm{Re}_D^{-0.5} \kappa_{ext}$$

Assuming that the extinction strain rate can be computed accurately for other fuels, the detachment velocity should now be predictable also if $t > 3\delta$

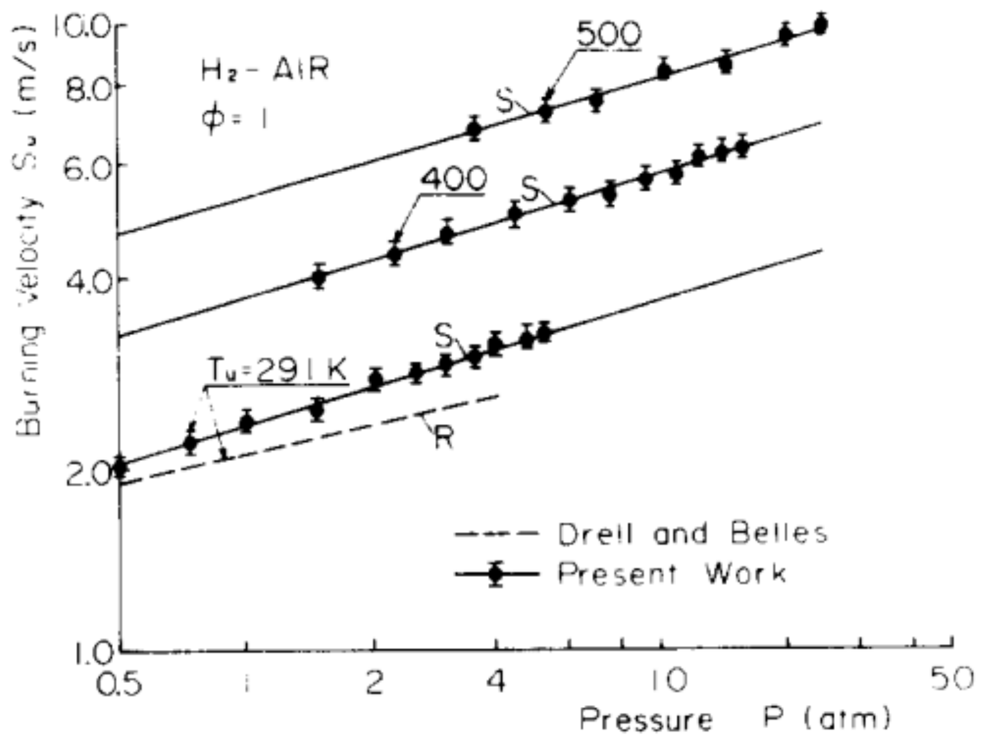
Guiberti et al. Combust. Flame 2019(203)

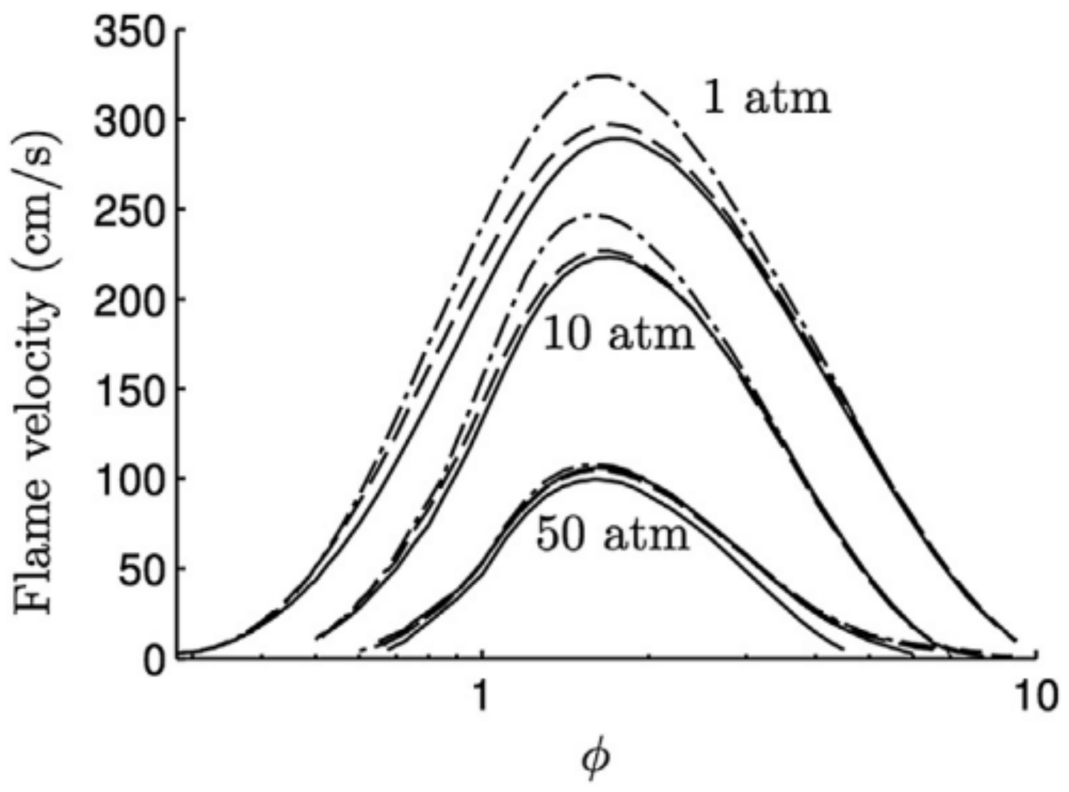
Flame detachment for H_2

$t < 3\delta$

↓

$$U_d = S_L/U_c \times f(\xi_{st})$$





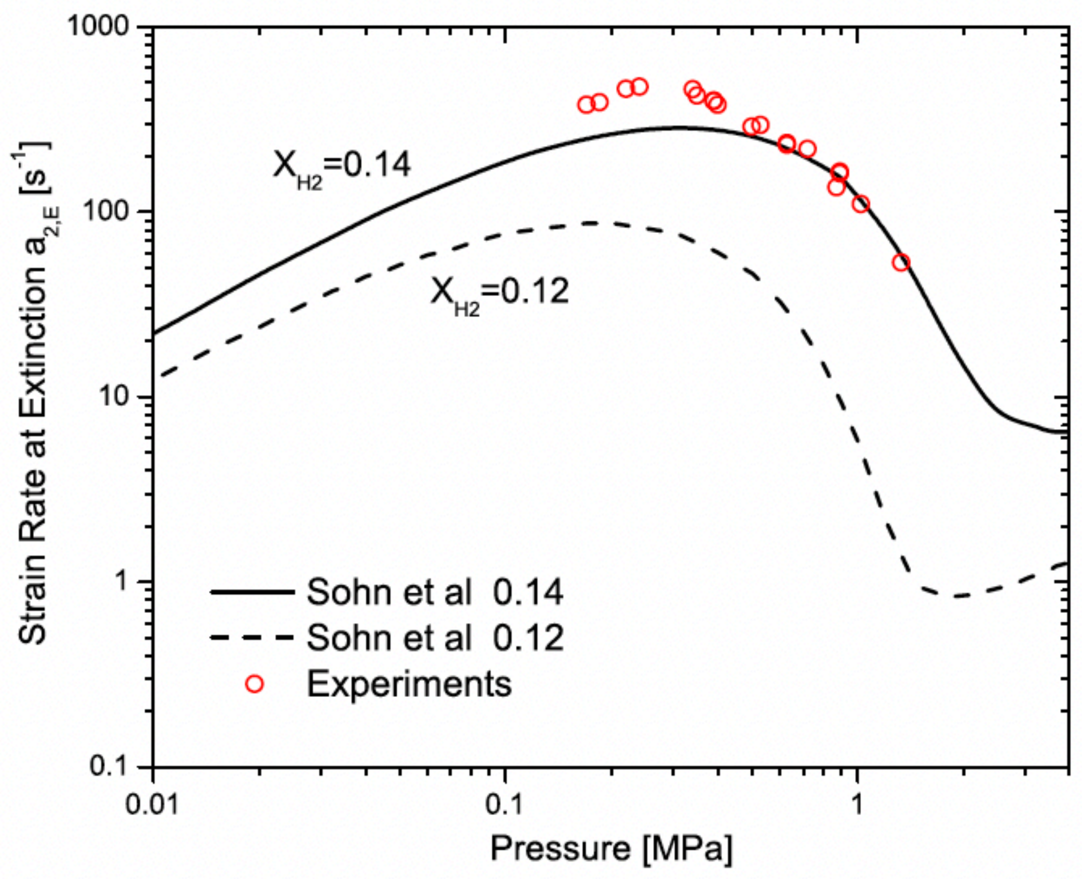
Iijima & Takeno Combust. Flame 1986(65) *Sanchez & Williams Prog. Energy Combust. Sci. 2014(41)*

$t = 3\delta$

$t > 3\delta$

↓

$$U_D = 128 D \mathrm{Re}_D^{-0.5} \kappa_{ext}$$



Niemann et al. Proc. Combust. Inst 2013(34)

At first, increasing pressure will retard detachment for H_2

But ξ_{st} is closer to the fast fuel jet for H_2, which promotes detachment

H_2 flames are very resistant to strain-induced extinction

Above some moderate pressure, detachment will be promoted for H_2

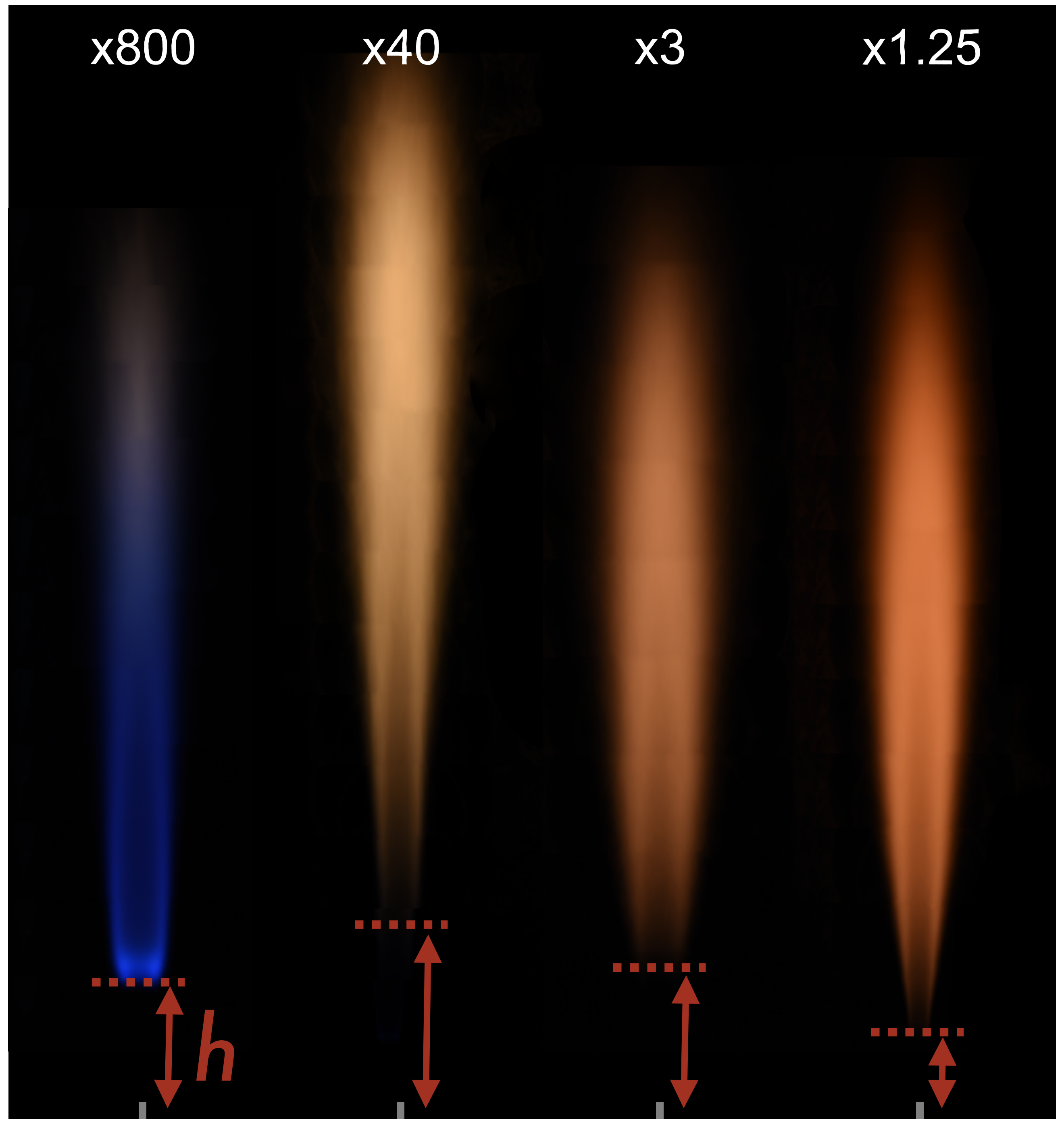
Guiberti et al. Combust. Flame 2019(203)

Lift-off height

Once detached and lifted, how far away from the nozzle is the flame base?

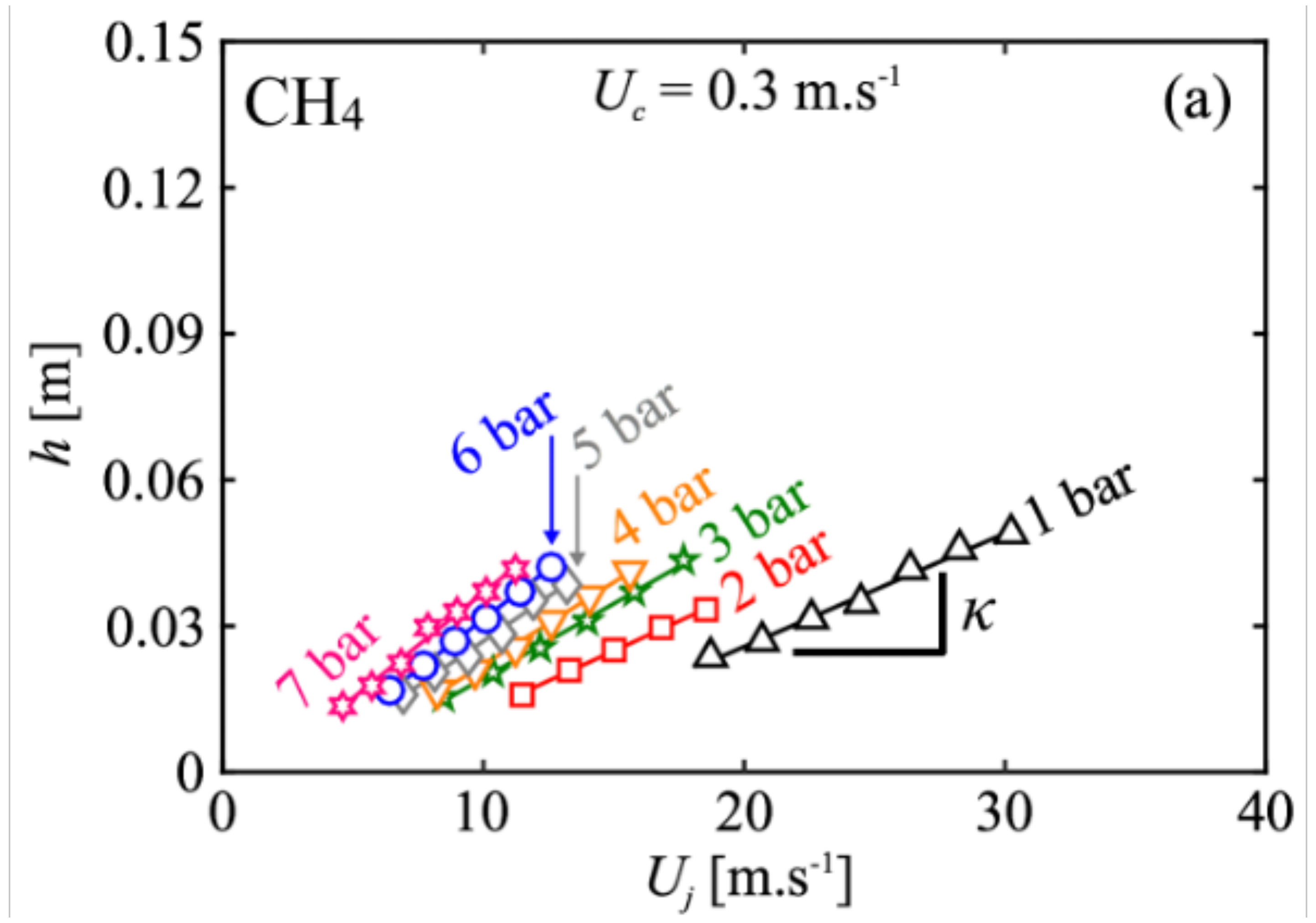
Lifted

Methane	Ethane	Methane	Ethane
1 bar	1 bar	7 bar	6 bar
U_j = 24 m.s^{-1}	15	10	13
U_c = 0.6 m.s^{-1}	0.6	0.3	0.6
Re = 4795	7593	13985	39485



Where are the conditions met for the leading edge of the flame to stabilize?

Lift-off height



Regardless of pressure, the *h* vs. *Uj* curves are linear

The lift-off height increases with the bulk jet velocity

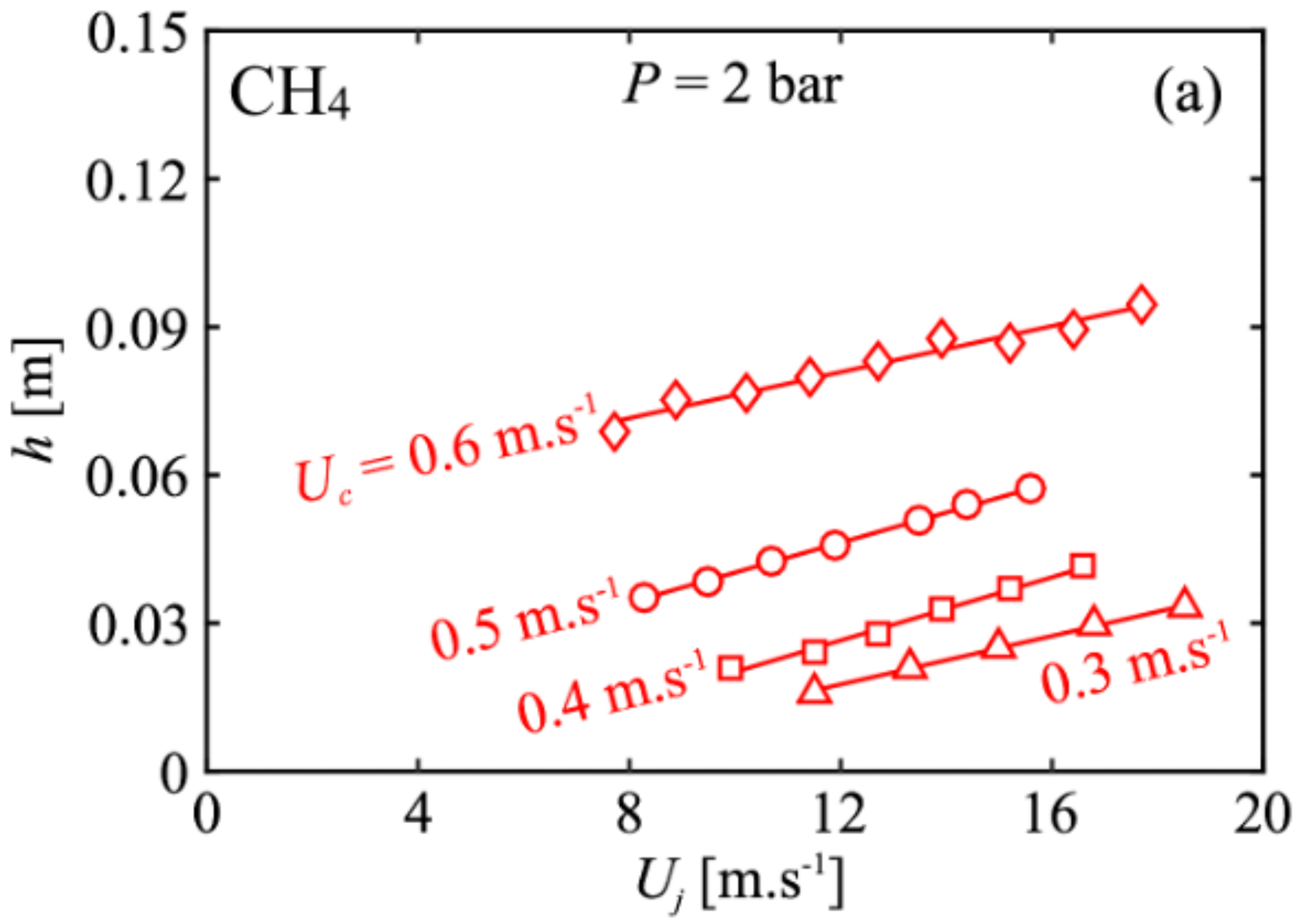
The lift-off height increases with pressure

The slope *K* is positive and is not too sensitive to pressure

If the co-flow velocity is increased to U_c = 0.6 m/s:

➡ The slope *K* decreases with pressure and can be negative

Lift-off height



The lift-off height increases with the co-flow velocity

At 2 bar, slope *K* does not depend on the co-flow velocity

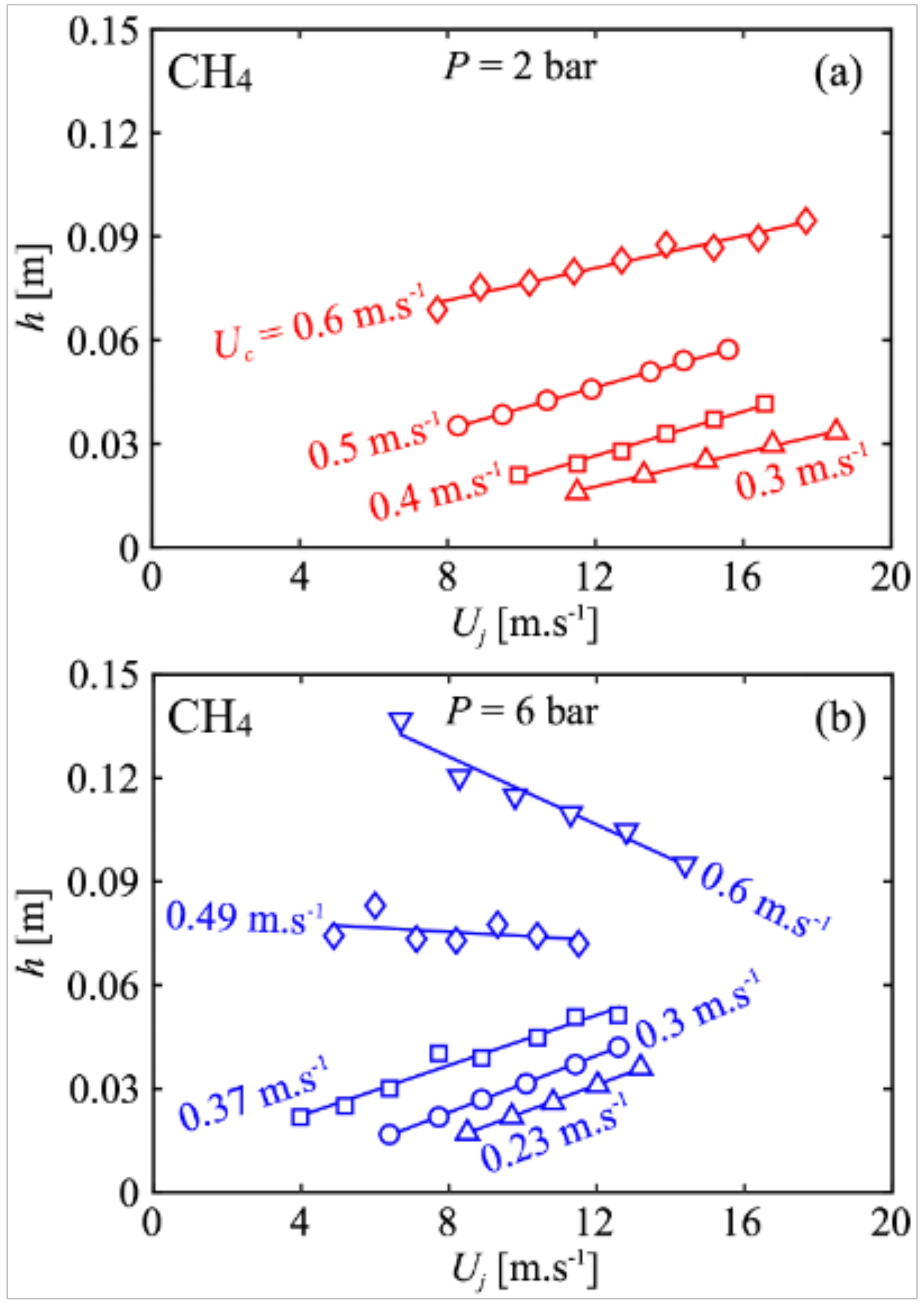
Further increasing the co-flow velocity leads to blow-off

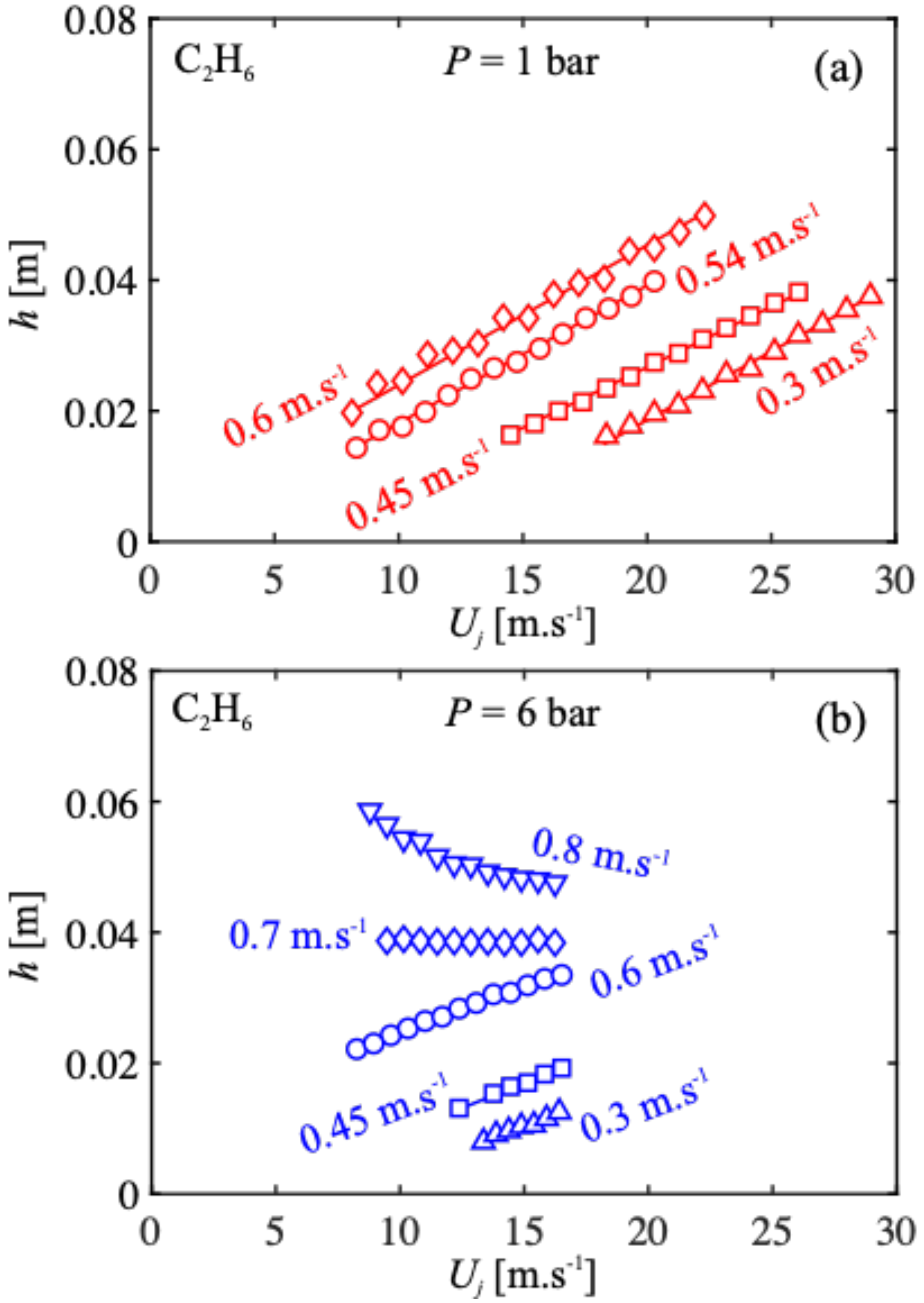
If the co-flow velocity exceeds a critical value:

➡ The slope *K* decreases with the co-flow velocity and can be negative

 Guiberti et al. Proc. Combust. Inst. 2019(37)

Lift-off height

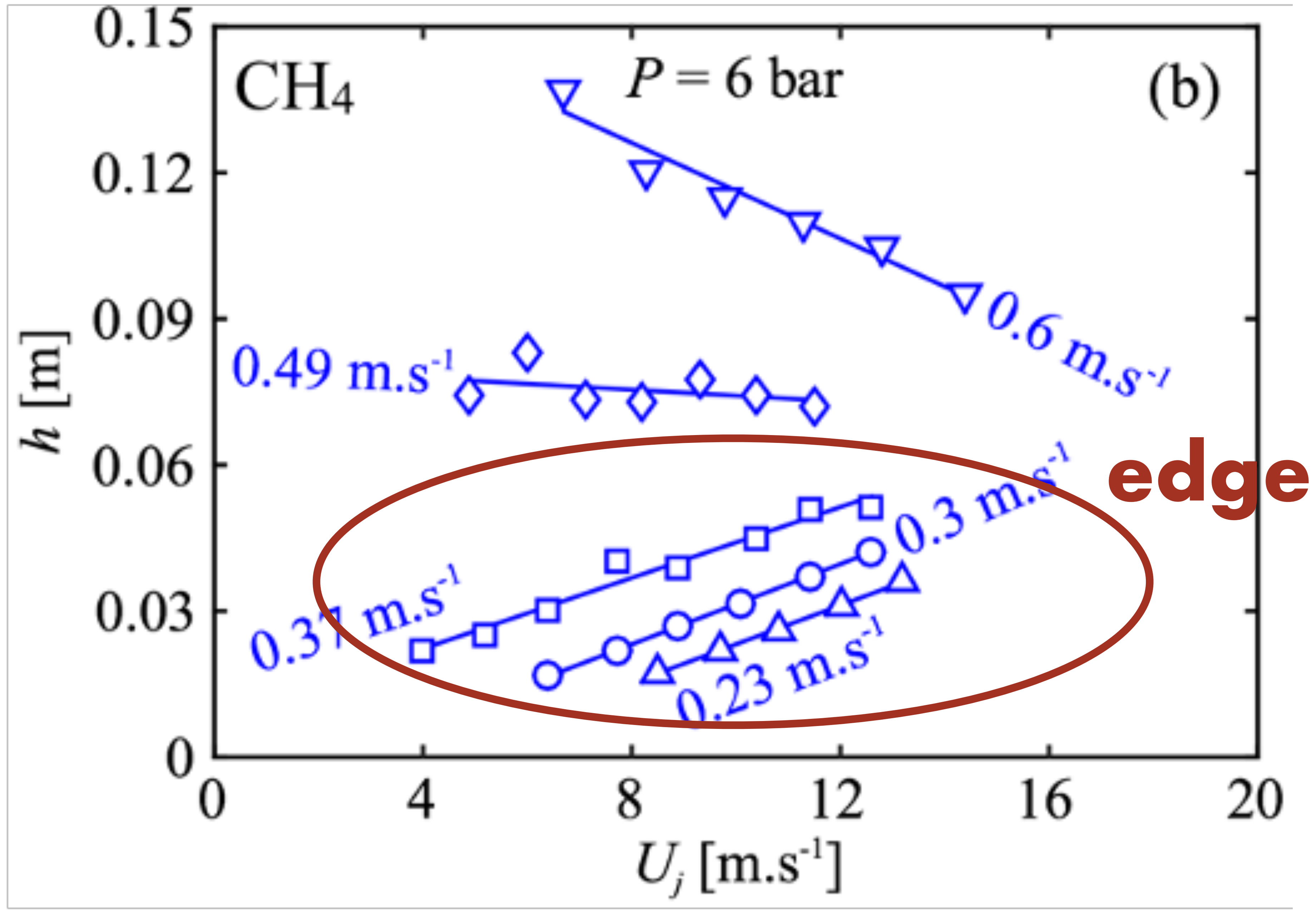




The same behavior is observed with ethane, albeit for a larger co-flow velocity

There seem to be a transition in the flame's stabilization mechanism if both pressure and co-flow velocity are large enough

Stabilization mechanisms



edge flames

- non-premixed flame sheet
- sits on a stoichiometric contour
- counters the incoming flow at a velocity close to the laminar burning velocity S_L

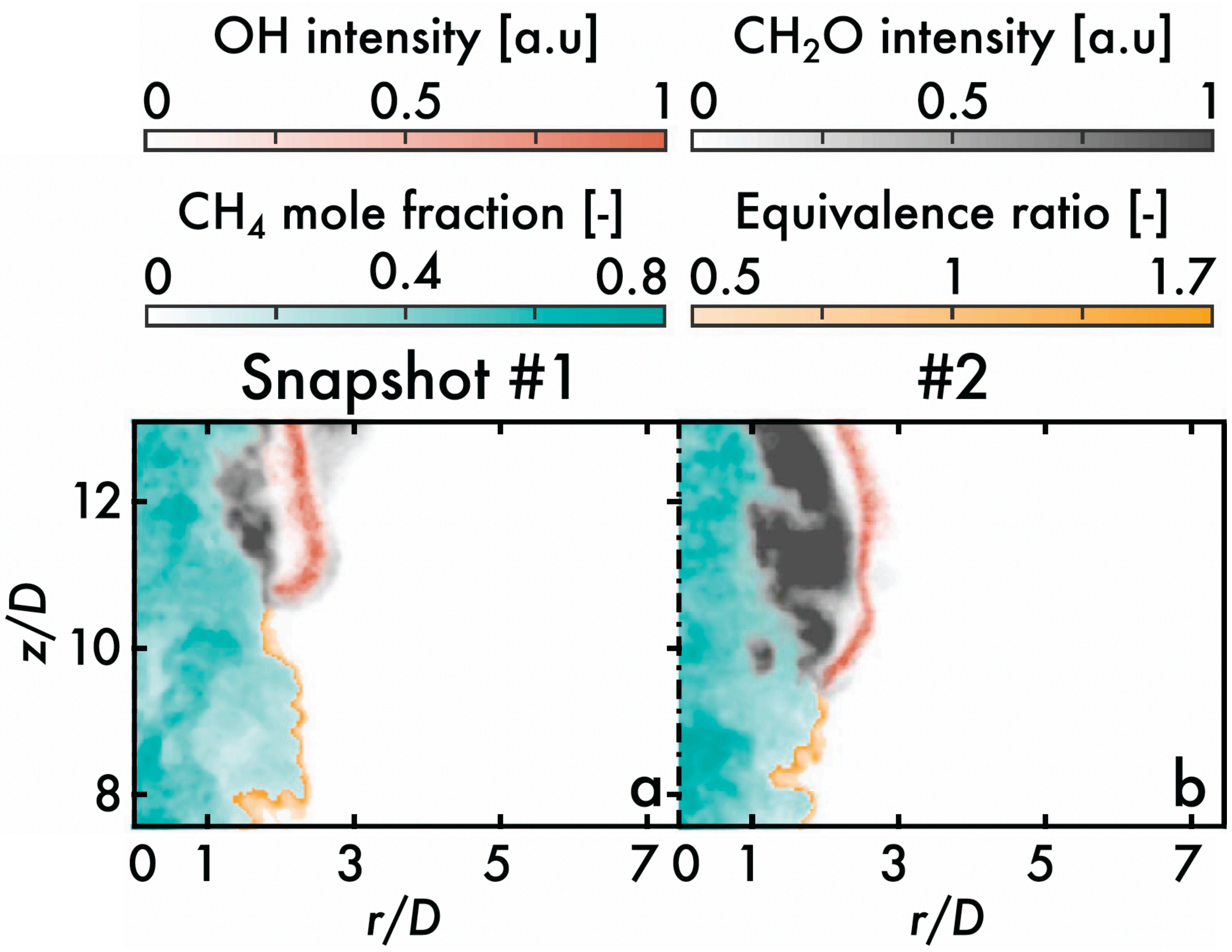
Chung S.H Proc. Combust. Inst. 2007
Li et al. Combust. Flame 2010
Karami et al. J. Fluid Mech. 2015

$\phi = 1 \;\&\; 0 < u < 3S_L$

More generally $0 < u < (\rho_u/\rho_b)^{1/2} S_L < 3S_L$ for air as the oxidiser

 Guiberti et al. Proc. Combust. Inst. 2019(37)

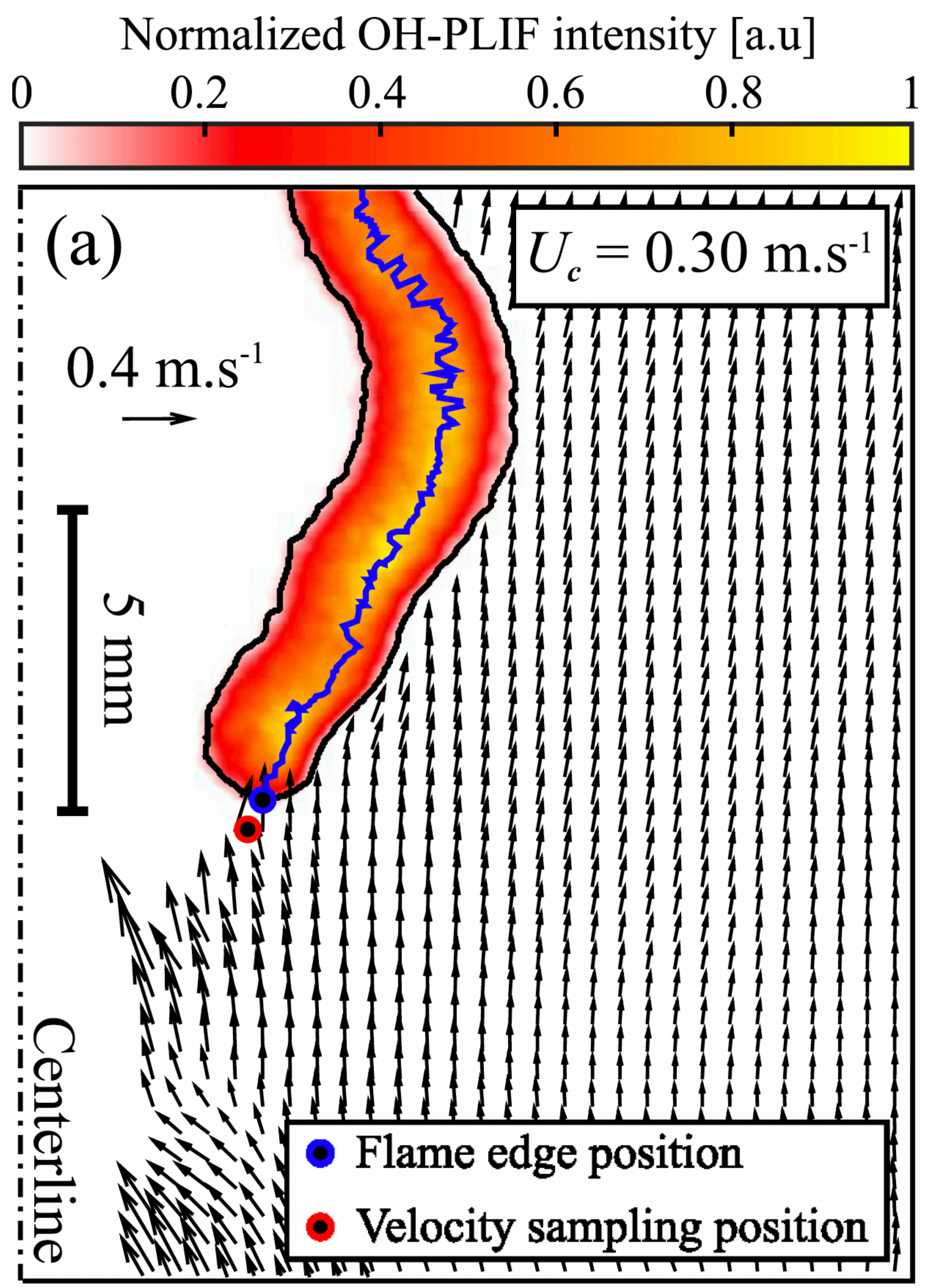
Stabilization mechanisms

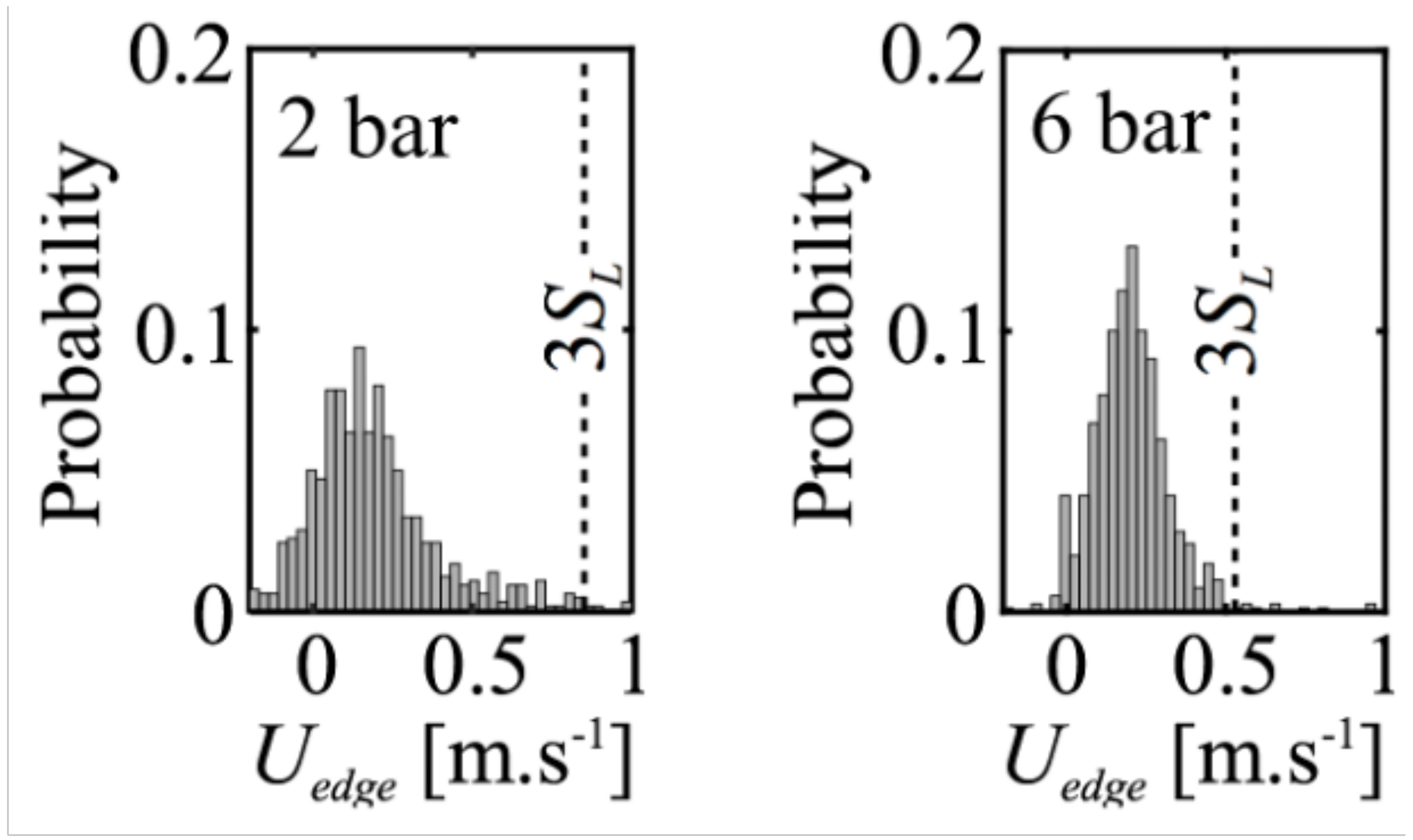


Multi-scalar imaging confirm the edge-flame structure at 6 bar and U_c = 0.3 m/s

Guiberti et al. Combust. Flame 2020(214)

Stabilization mechanisms

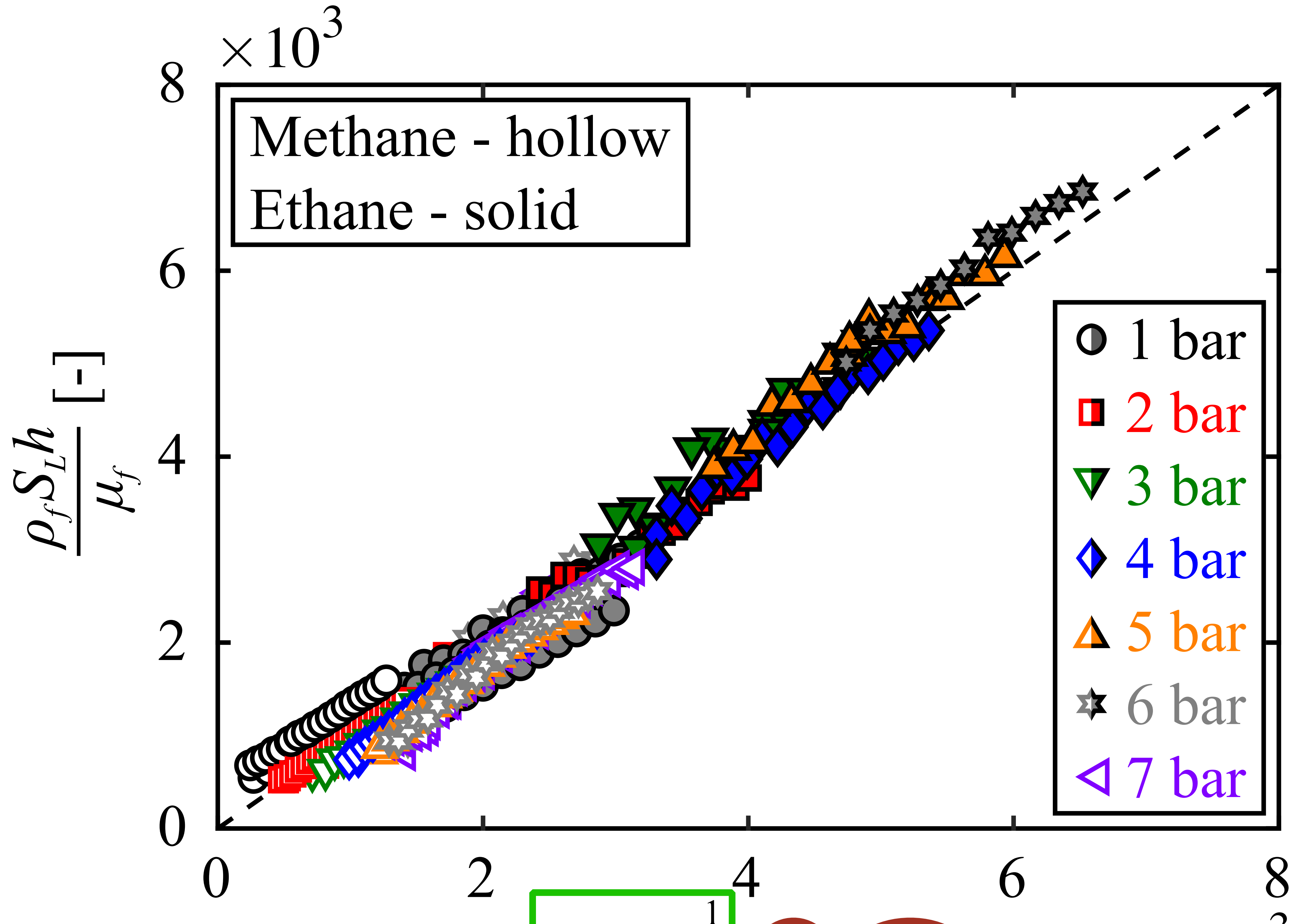




Combined velocimetry (PIV) and OH-PLIF confirm edge-flame stabilization

Stabilization mechanisms

Can we predict the lift-off height for wide ranges of fuel, pressure, co-flow, geometry, ...?



$$50\frac{U_j + \frac{1.5\left(\frac{\rho_o}{\rho_f}\right)^{\frac{1}{2}}(U_c+1.5S_L)}{Sc \cdot Z_{st}}}{S_L} g(\bar{\rho})\ [-]$$

A non-dimensional lift-off height is defined

Kalghatgi et al. Combust. Sci. Technol. 1984

It can be predicted well by a physics-based model, which features quantities that can be easily computed

h increases if U_j increases

h decreases if S_L increases

The co-flow pushes the flame downstream

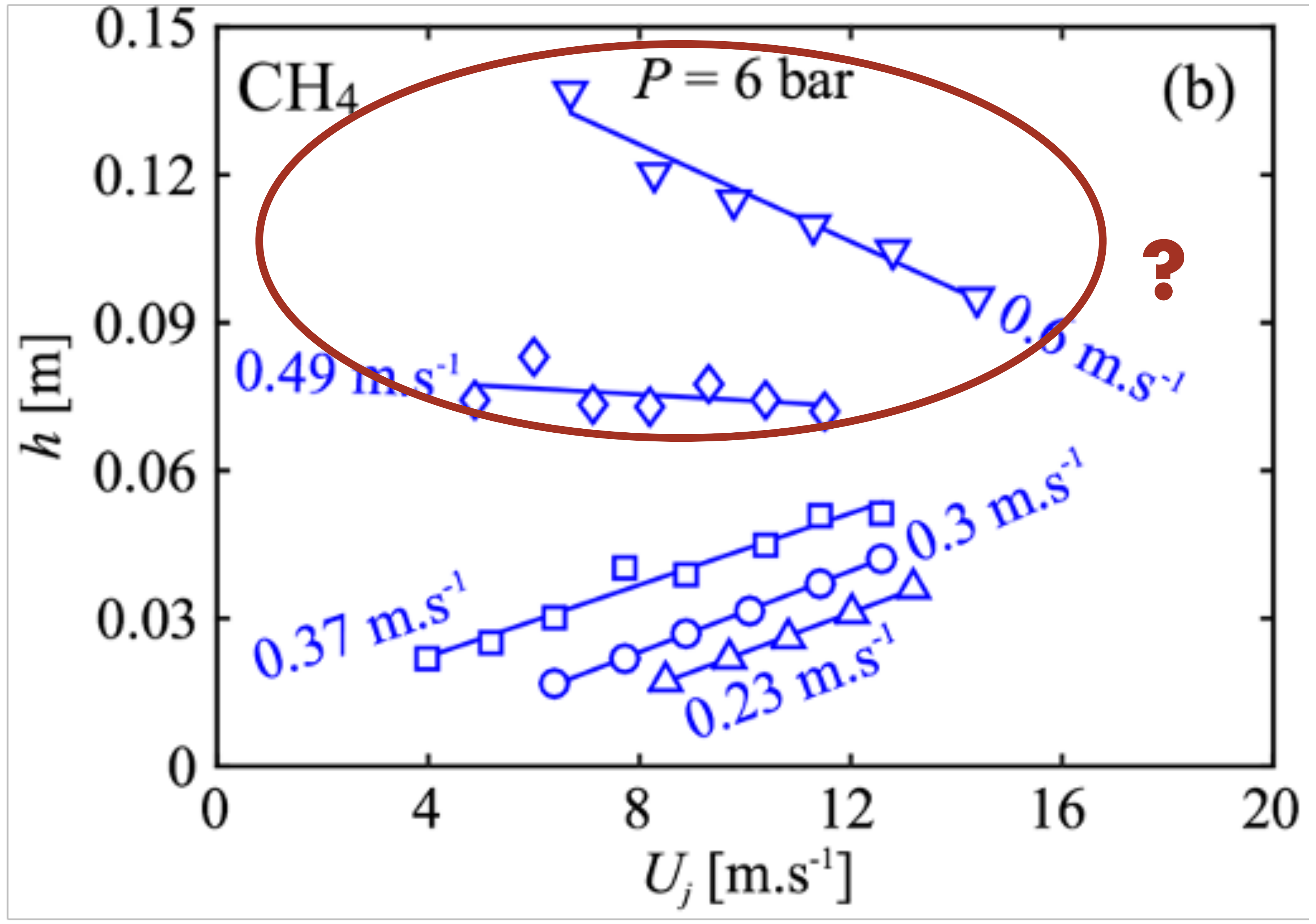
- *Mixing via Kelvin-Helmholtz instabilities depends on the density ratio*
- *The stoichiometric mixture fraction controls how influential the co-flow is*
- *A turbulent Schmidt number accounts for velocity and species spread rates*

A corrective term allows for a negative Y-intercept of the h vs. U_j curve

Upatnieks Combust. Flame 2004
Han and Mungal Combust. Flame 2003
Montgomery et al. Proc. Combust. Inst. 1998
Kalghatgi Combust. Sci. Technol. 1984

Guiberti et al. Combust. Flame 2019(219)

Stabilization mechanisms



What is the critical co-flow velocity above which inversion occurs?

Fuel	Pressure (bar)	U_c^{crit} (K = 0) (m/s)	U_c^{crit}/S_L (-)
Methane	3	0,6	3
Methane	6	0,48	3,2
Methane	7	0,43	3,0
Ethane	6	0,70	3,2
Ethylene	1	2,0	3

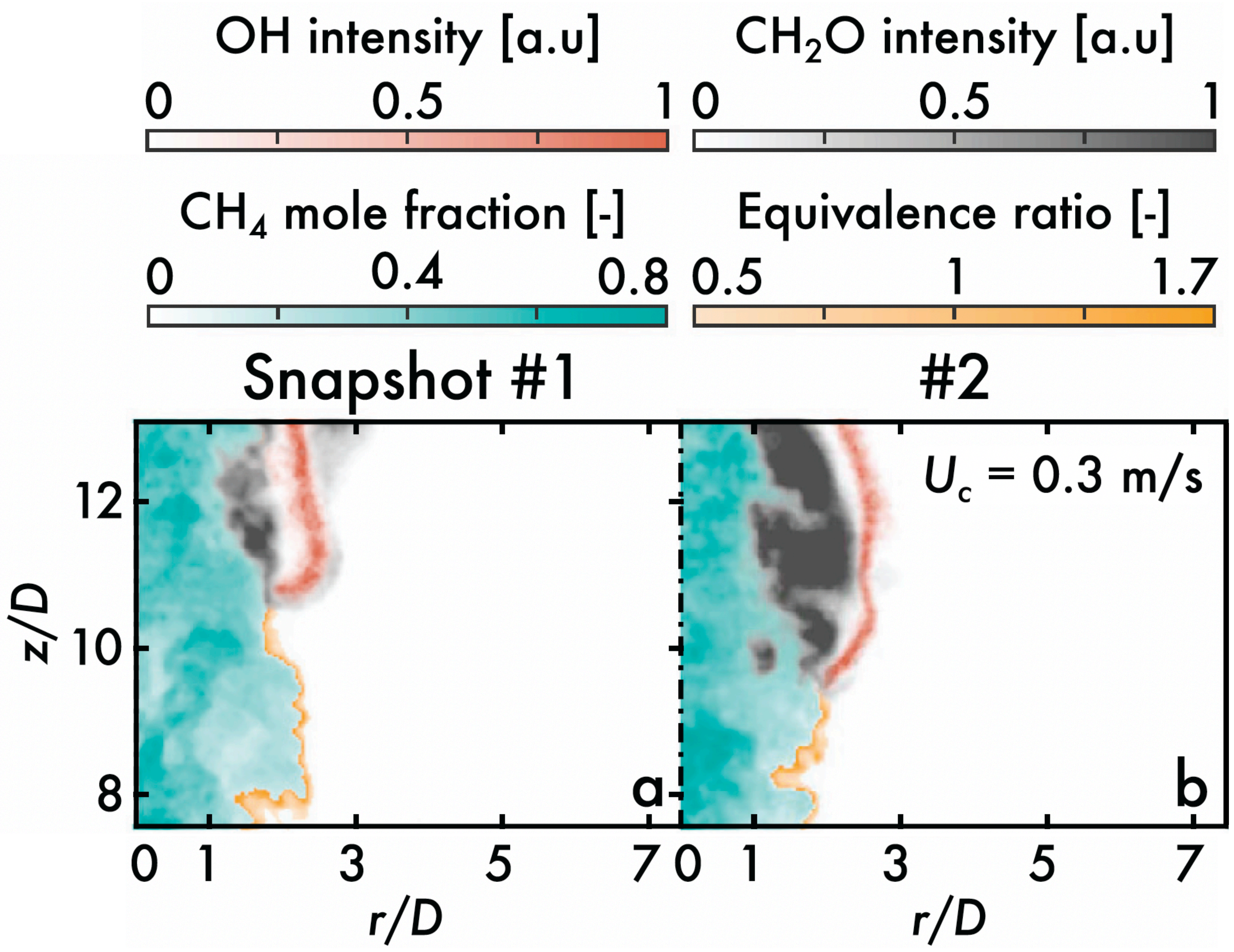
The critical co-flow velocity above which an edge flame cannot stabilize is $U_c^{crit} = 3S_L$

This is consistent with the experimental evidence of a maximum edge-flame speed of $3S_L$

What happens if $U_c > U_c^{crit} = 3S_L$?

Guiberti et al. Combust. Flame 2020(214)
Brown et al. Combust. Sci. Technol. 2010

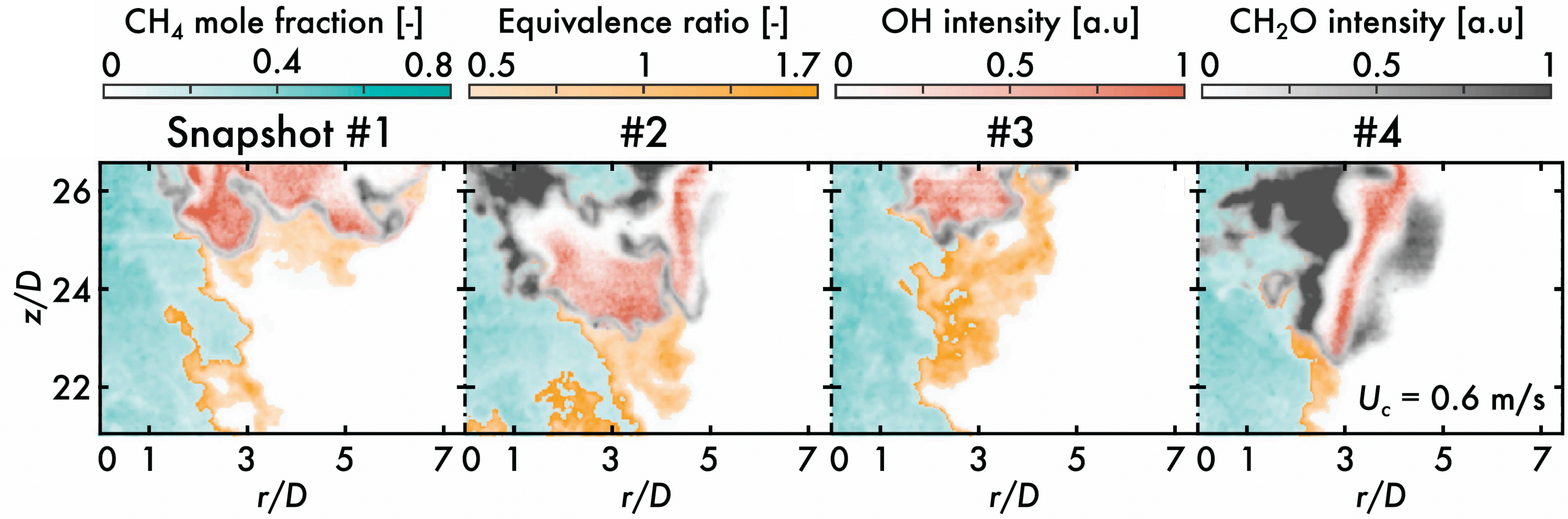
Stabilization mechanisms



Guiberti et al. Combust. Flame 2020(214)

Stabilization mechanisms

If the co-flow velocity is increased to U_c = 0.6 m/s (U_c^{crit} = 0.5 m/s):



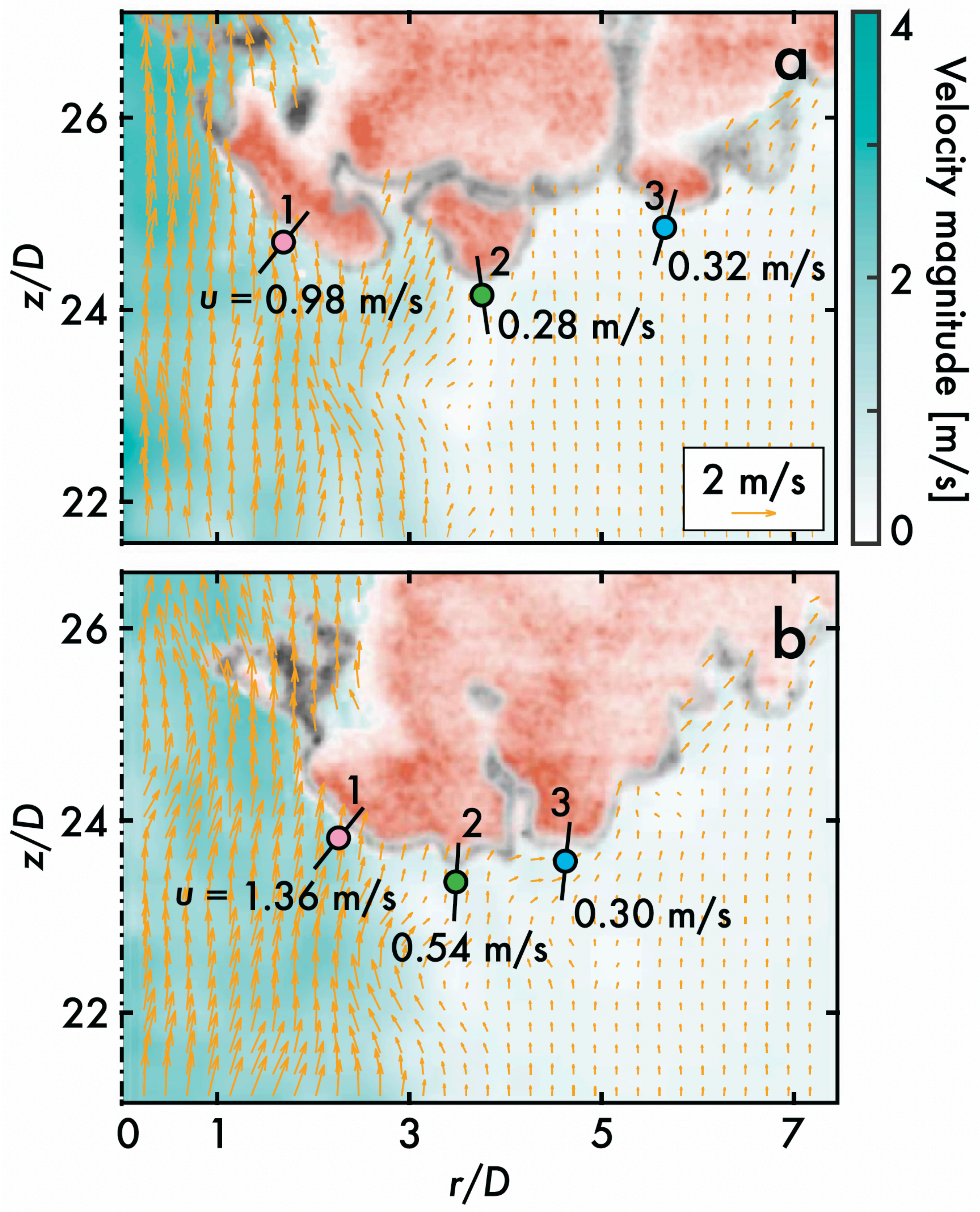
➡ The flame is pushed further downstream, where the width of the flammable zone has increased significantly due to sufficient mixing

➡ The structure of the flame becomes vastly different

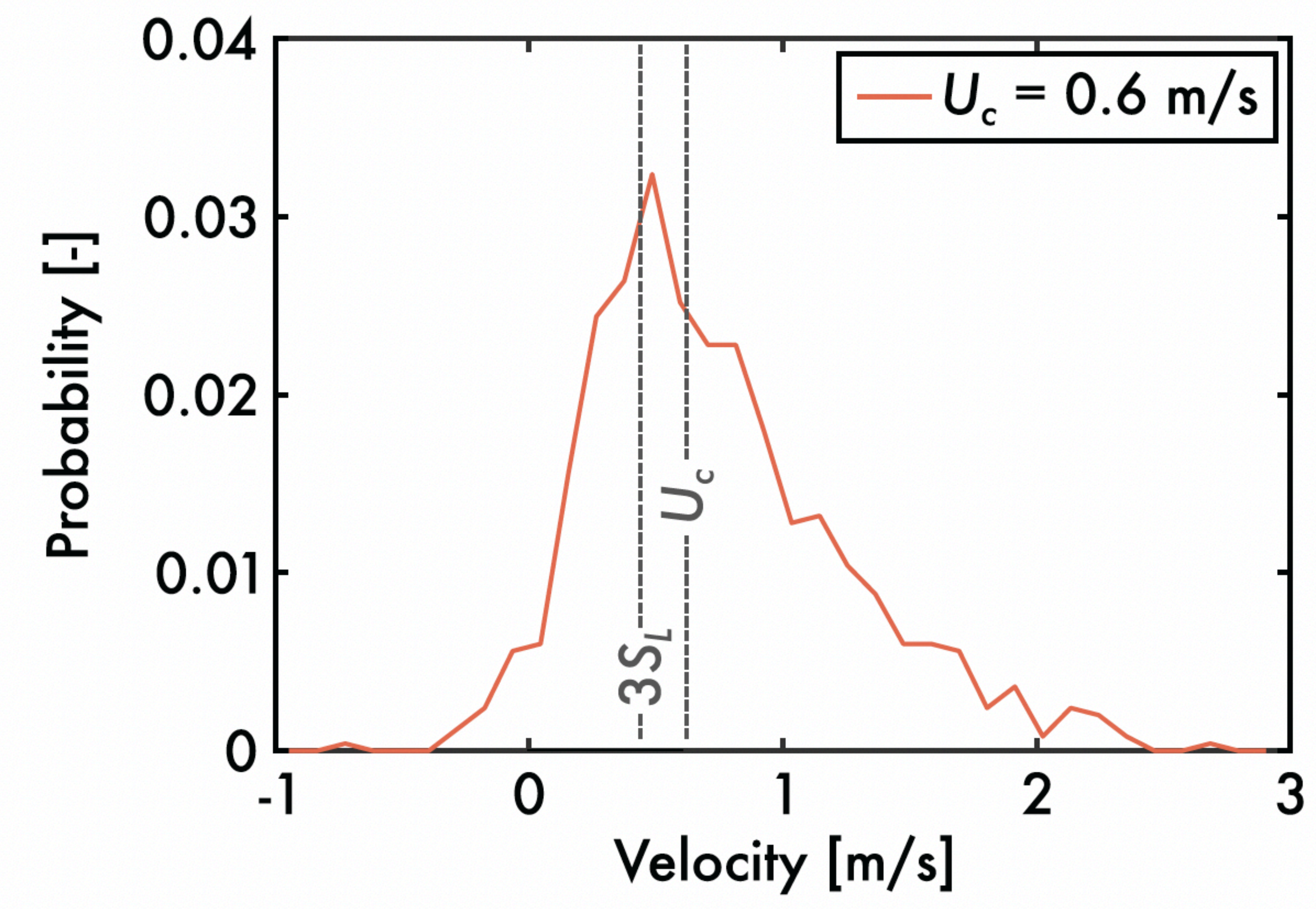
 Guiberti et al. Combust. Flame 2020(214)

Stabilization mechanisms

If the co-flow velocity is increased to U_c = 0.6 m/s (U_c^{crit} = 0.5 m/s):



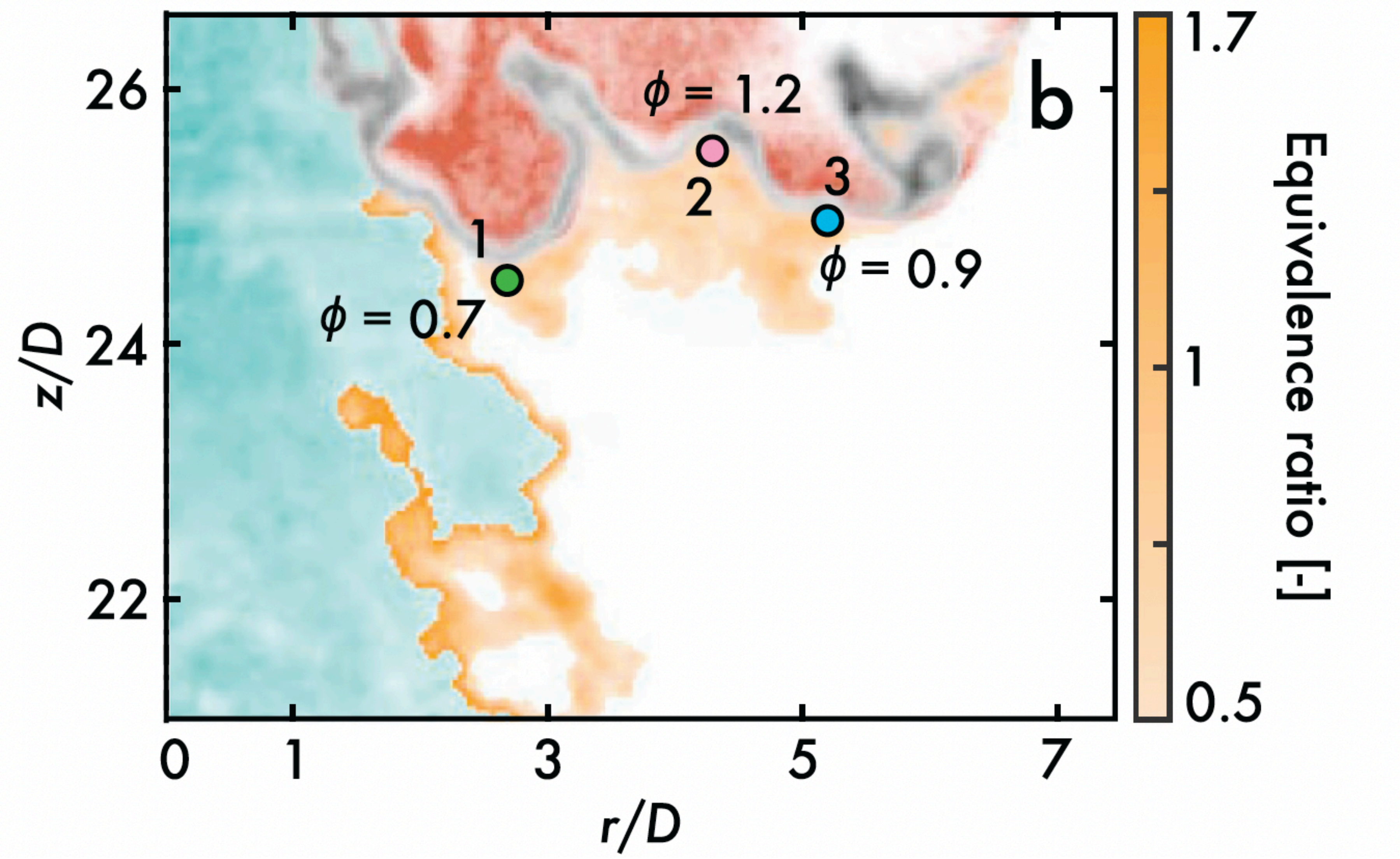
The normal velocity immediately upstream of the flame front may exceed that possible with an edge flame



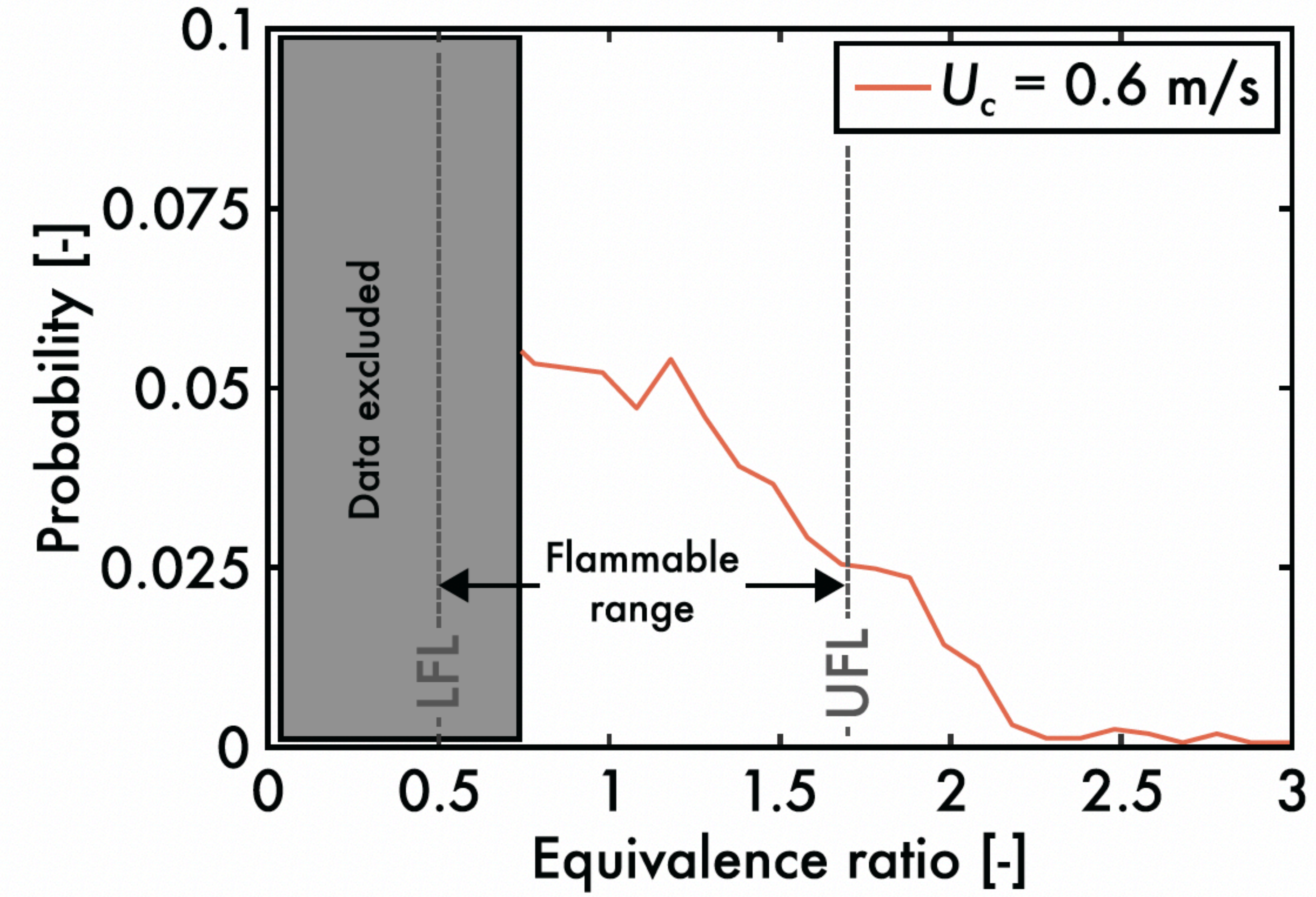
Guiberti et al. Combust. Flame 2020(214)

Stabilization mechanisms

If the co-flow velocity is increased to U_c = 0.6 m/s (U_c^{crit} = 0.6 m/s):



The equivalence ratio immediately upstream of the flame front spans the whole flammable range



These observations are consistent with turbulent premixed flame stabilization

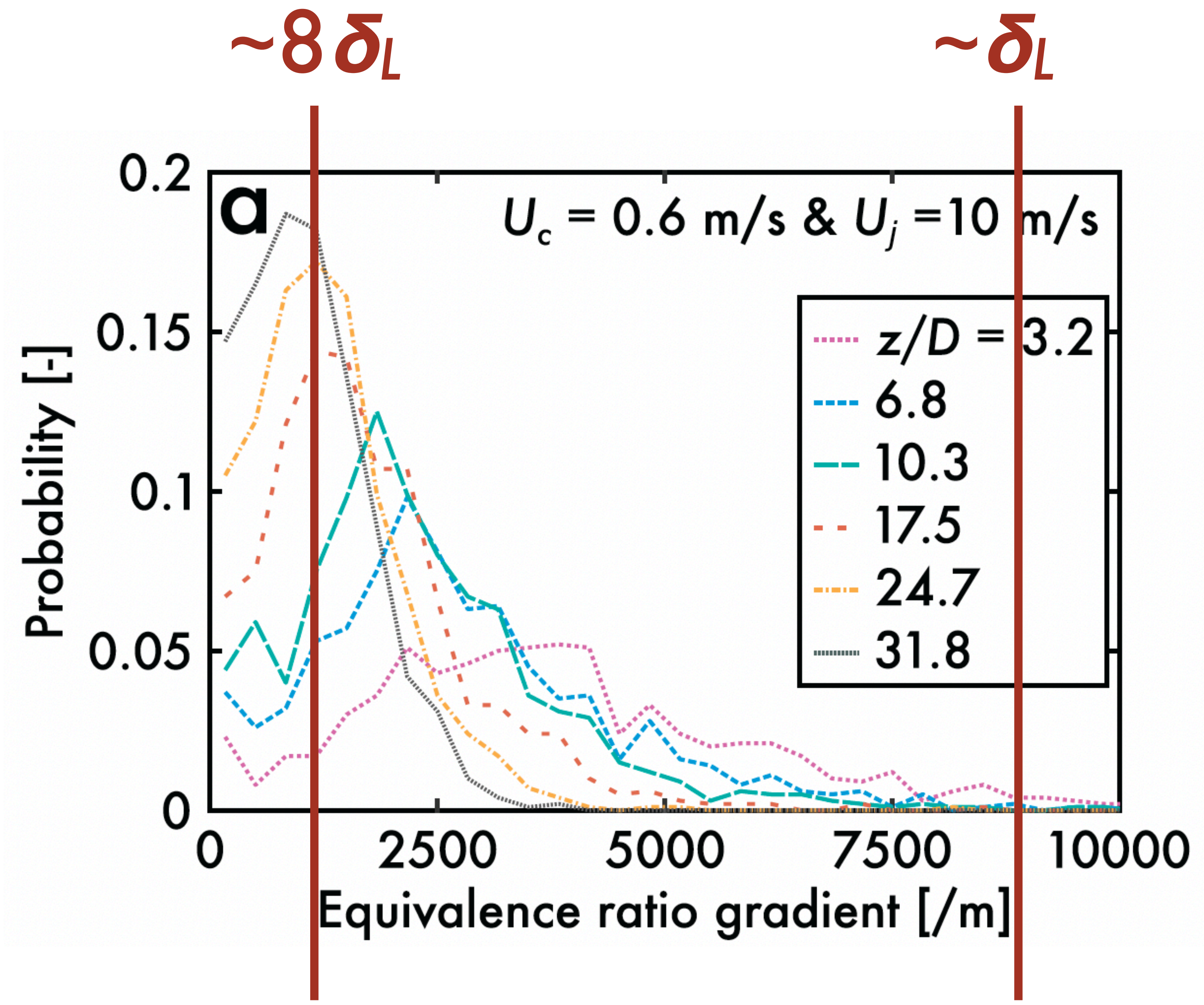
Guiberti et al. Combust. Flame 2020(214)

Stabilization mechanisms

How far from the nozzle does a flame needs to be to exist as a premixed flame?

This can be partially answered by considering gradients of equivalence ratio and the laminar thermal flame thickness δ_L

Spans the flammable range over:



Turbulent mixing and equivalence ratio gradients provide a lower bound of the lift-off height

The exact lift-off height also depends on the turbulent burning velocity

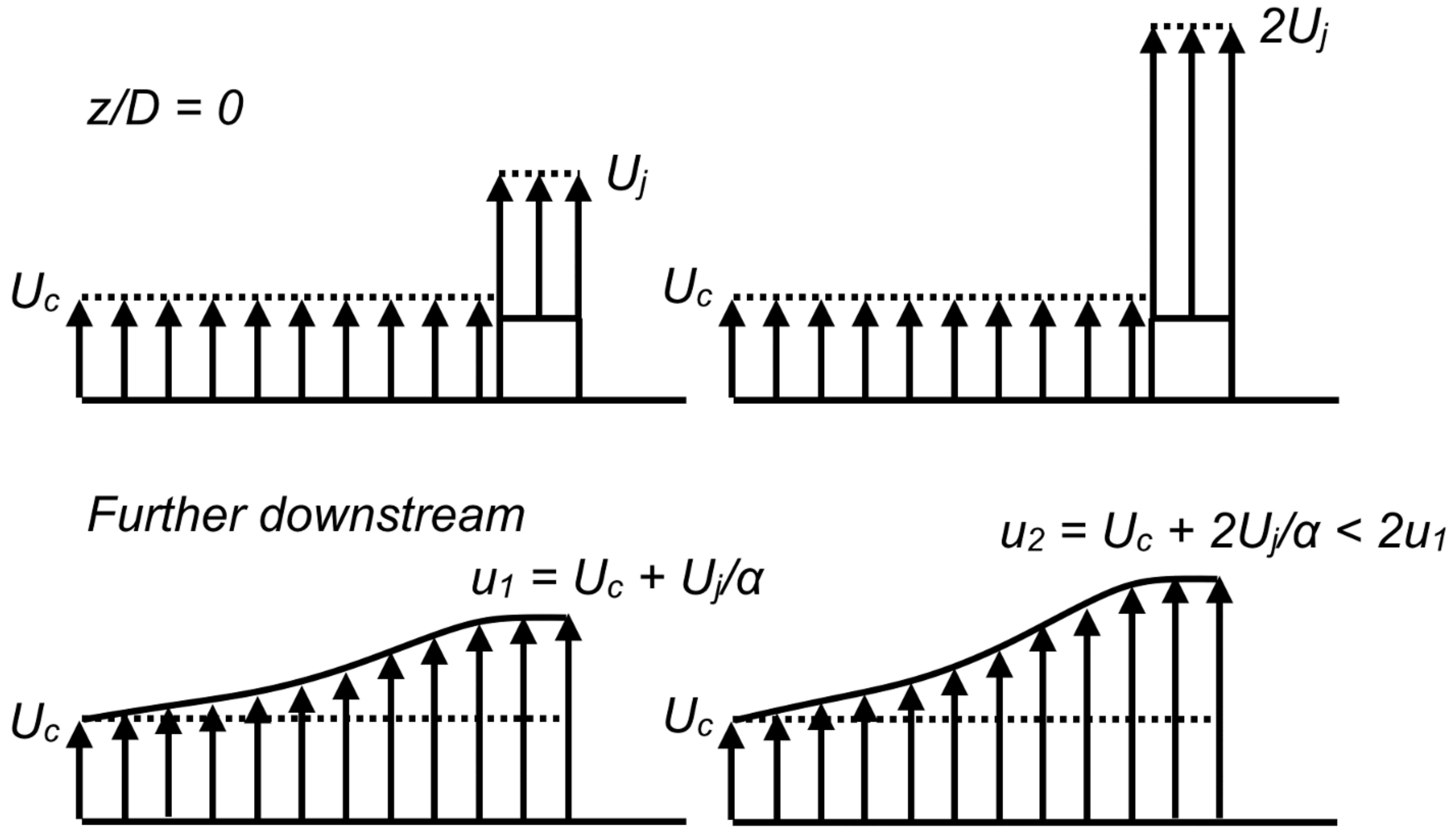
Guiberti et al. Combust. Flame 2020(214)

Stabilization mechanisms

The turbulent burning velocity may be calculated using a model such as:

$$S_T = S_L + 0.62 {S_L}^{1/2} u'^{1/2} \left(\frac{u' L_T}{\upsilon} \right)^{1/4} \quad \propto U_j^{3/4}$$

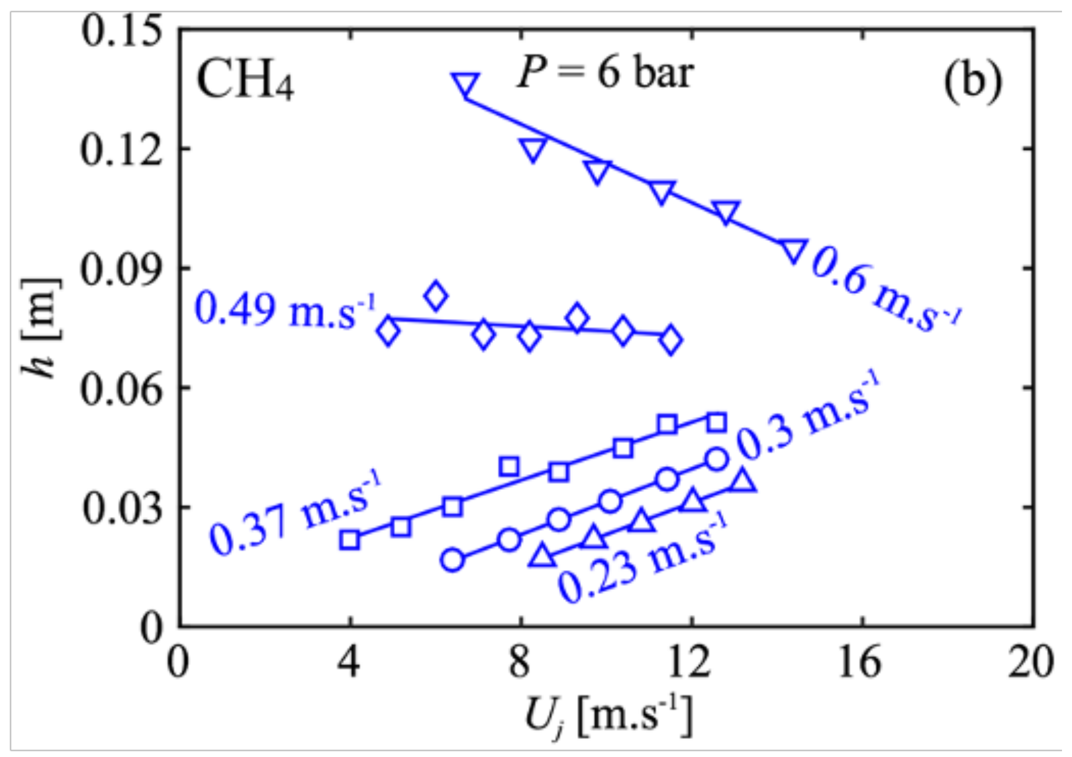
Gulder Proc. Combust. Inst. 1991



Adapted from: *Brown et al. Combust. Sci. Technol. 2010*

If U_c is sufficiently large, S_T increases faster than the local velocity u when the U_j is increased

➡ The flame propagates closer to the nozzle



Guiberti et al. Combust. Flame 2020(214)

Stabilization mechanisms

Specifically, the effects of pressure are:

- For hydrocarbons, S_L decreases with *P*. Therefore, the critical co-flow velocity decreases with *P* too

  ➡ What about H_2 that features a non-monotonic pressure sensitivity?

- Once pushed downstream, the flame may blow-out, or stabilize as a premixed flame

  ➡ Increasing *P* enhances mixing, which helps to stabilize the flame and retards blow off

  ➡ This is why slope inversion is easier to observe at elevated pressure or with fast fuels (H_2?)

Guiberti et al. Combust. Flame 2020(214)

Conclusions for the stabilization of non-premixed flames

The pressure knob allowed us to refine our understanding of the mechanisms controlling the detachment and lift-off height of turbulent non-premixed flames

We can predict the conditions leading to the detachment of these flames **H_2? Swirl?**

We can predict if lifted flames are propagating as edge flames or premixed flames **H_2? Swirl?**

If they are edge flames, we can predict their lift-off height **H_2? Swirl?**

Diagnostics opportunities for H_2 at high pressure

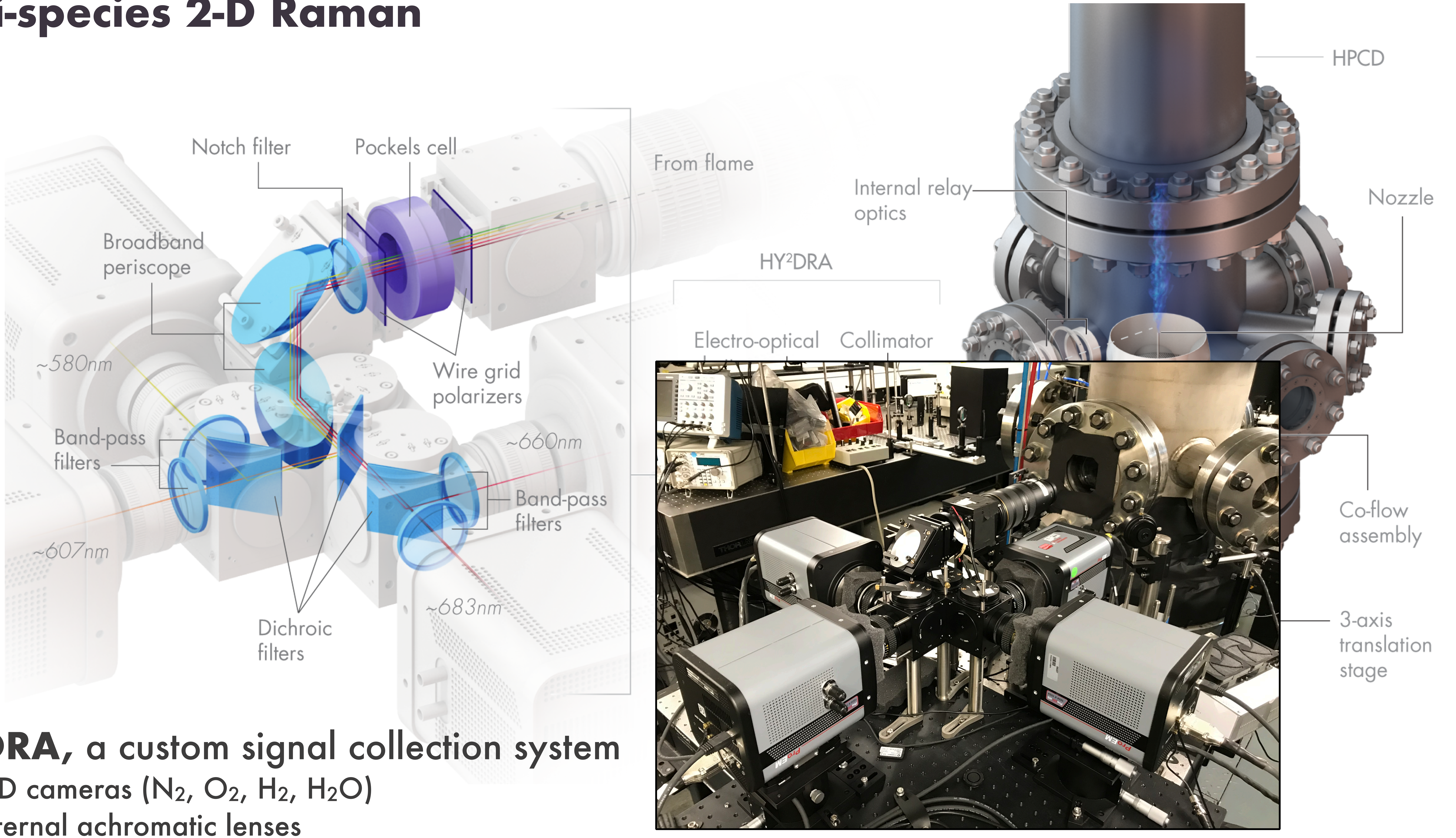
H_2 is a simple fuel: less scalars need to be measured to capture the flame chemistry

The increase of number density due to an increase of pressure may yield more intense signals

➡ **Demonstrate the first simultaneous single-shot imaging of all major species, OH, mixture fraction, and temperature in a turbulent flame**

Guiberti et al. Proc. Combust. Inst. 2021(38)

Multi-species 2-D Raman



HY²DRA, a custom signal collection system

- 4 CCD cameras (N_2, O_2, H_2, H_2O)
- 4″ internal achromatic lenses
- Pockels cell electro-optical shutter
- Advanced dichroic mirror assembly

Guiberti et al. Proc. Combust. Inst. 2021(38)

Multi-species 2-D Raman

The Raman signal intensity is a function of number density $n(X_k,T)$

Therefore, one has 2 options:

(1) also **measure temperature** (e.g. with Rayleigh) and derive X_k from single species Raman using the **ideal gas law**

(2) **measure all major species** with Raman and use additional equation $\sum X_k = 1$ to infer temperature

Because all major species and temperature are measured, **OH-PLIF is made quantitative** by computing **quenching rates** and **Boltzmann population distributions**

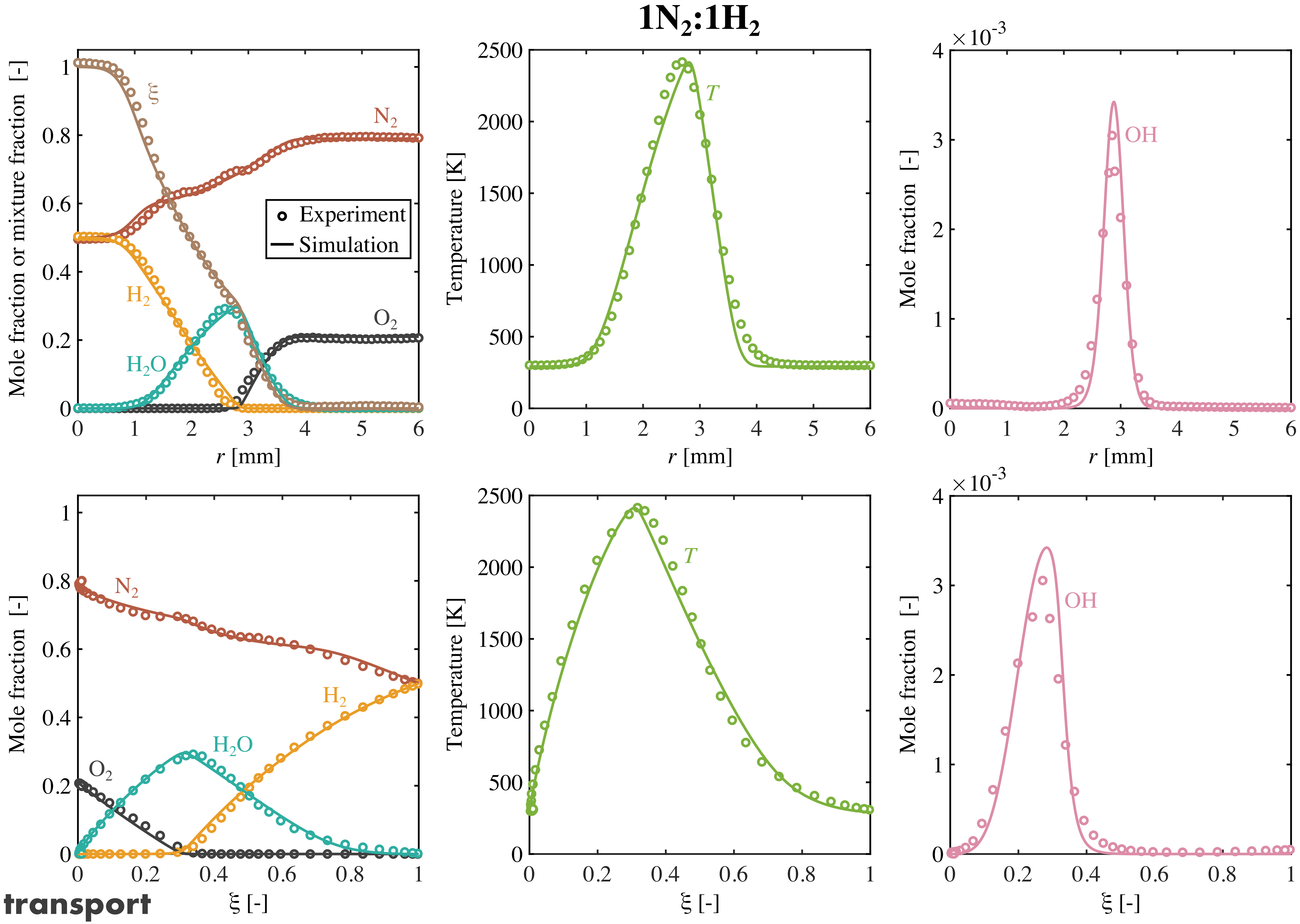
Guiberti et al. Proc. Combust. Inst. 2021(38)

Multi-species 2-D Raman

Results of the calibration in laminar N_2:H_2 non-premixed jet flames at 12 bar

1 row of pixels

Averaged over 100 shots

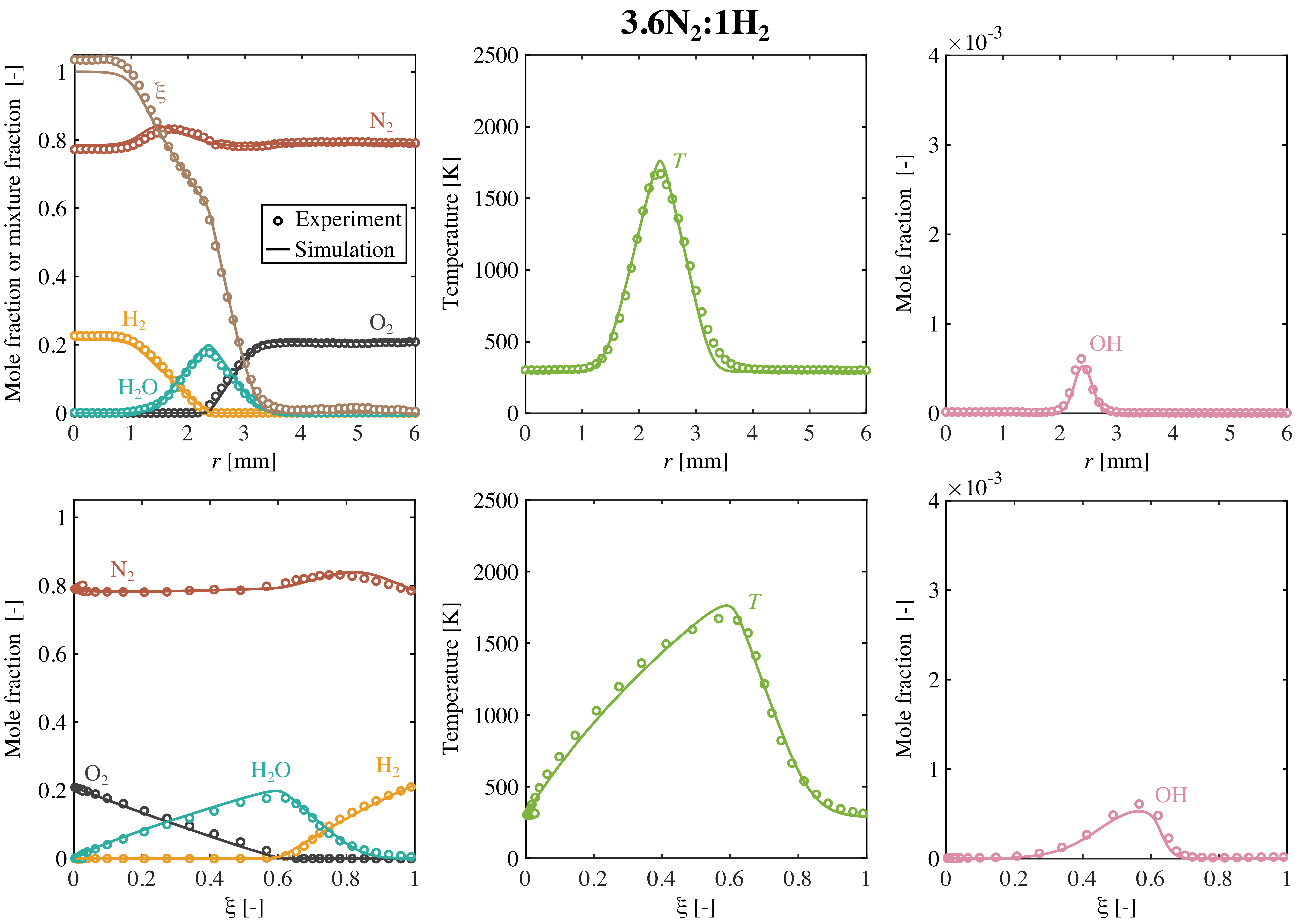


Simulations

- Chemkin
- Opposed-flow
- USCII mech
- **Multicomponent transport**

Multi-species 2-D Raman

Results of the calibration in laminar N_2:H_2 non-premixed jet flames at 12 bar



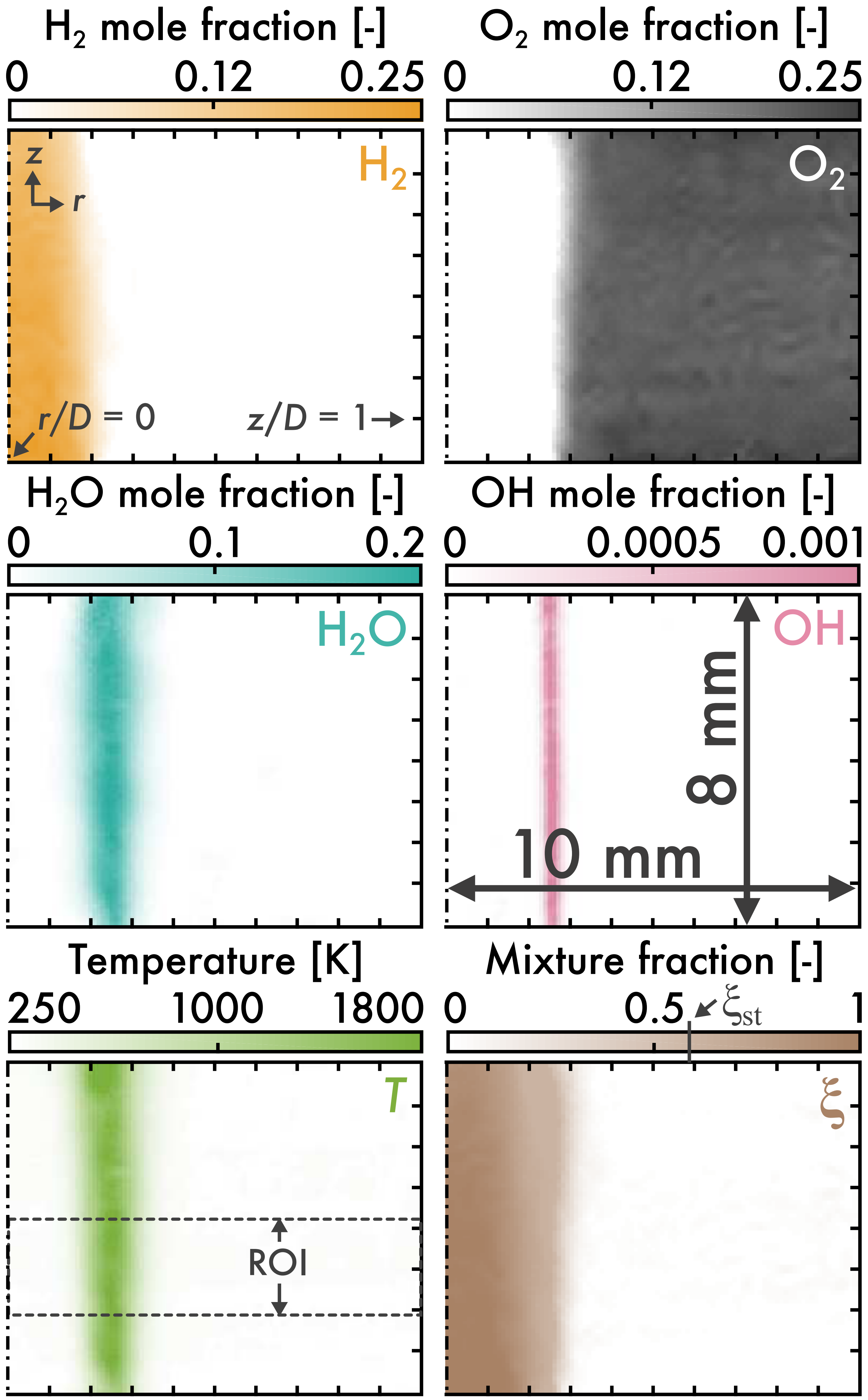
Accuracy

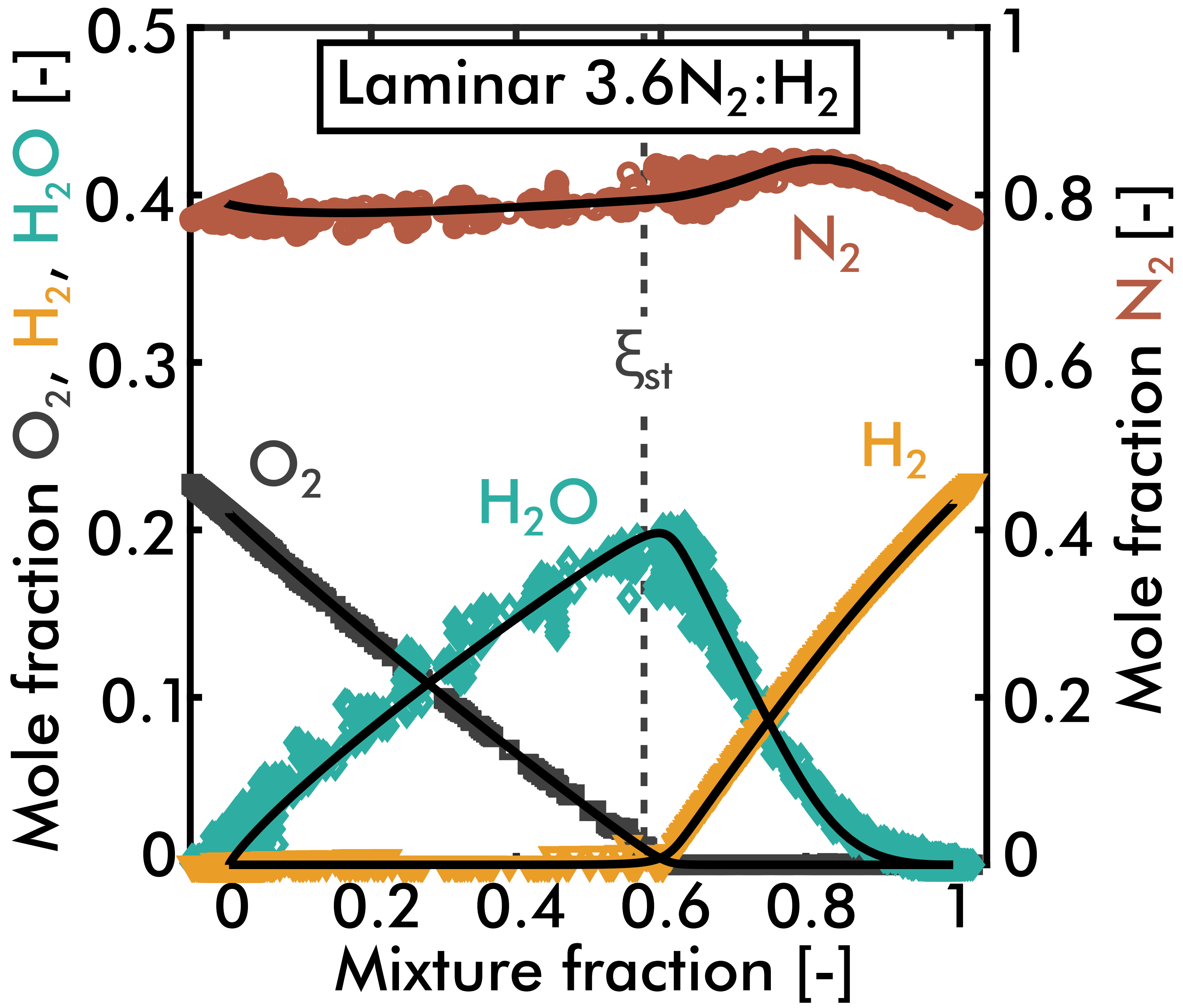
N_2	2 %
O_2	2 %
H_2	4 %
H_2O	10 %
ξ	5 %
OH	10 %
T	5 %

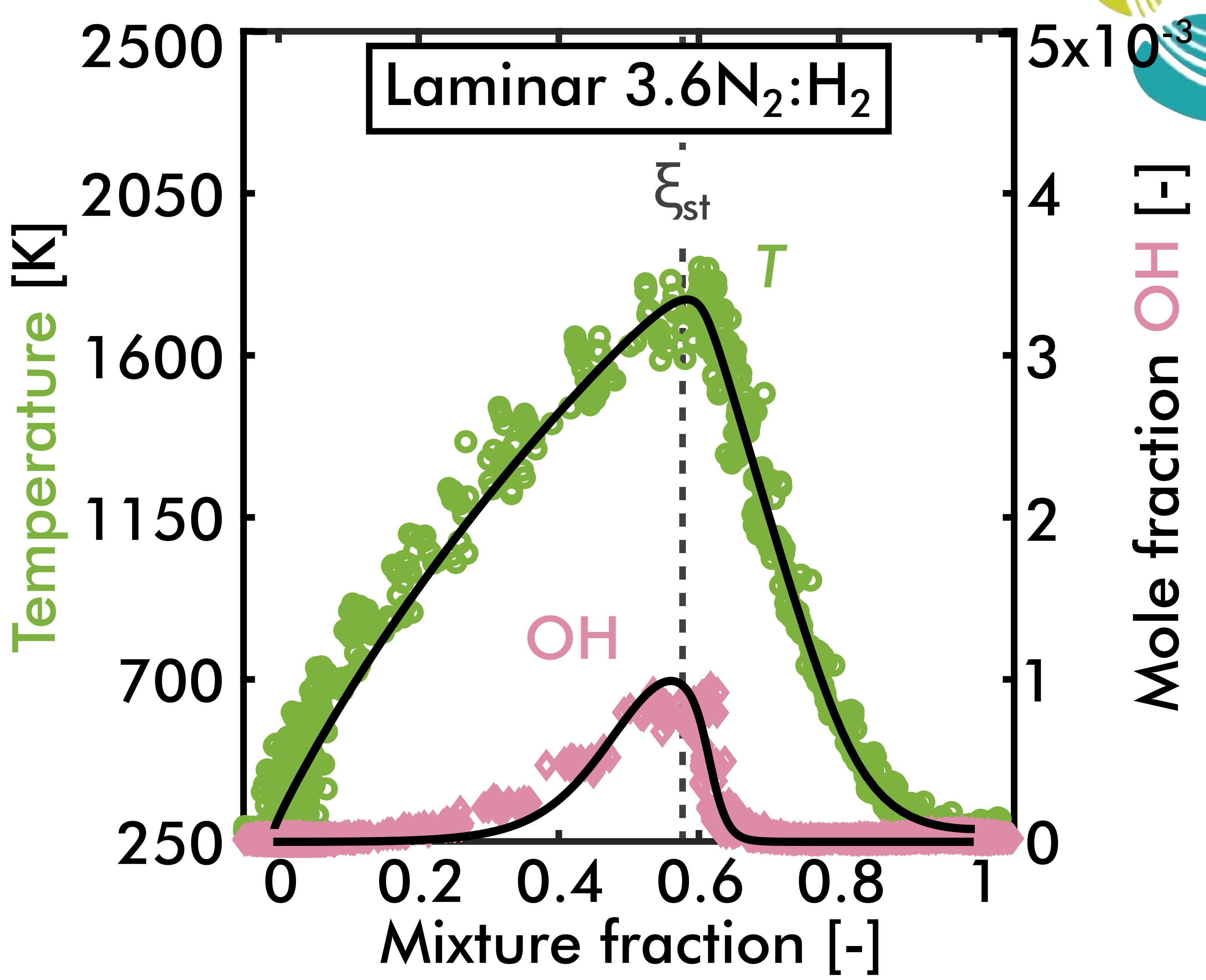
Precision

N_2	2 %
O_2	3 %
H_2	4 %
H_2O	6 %
ξ	5 %
OH	10 %
T	5 %

Multi-species 2-D Raman







Single shot - all pixels in ROI

We accurately capture the **full thermo-chemical structure** of the flame in a **single shot**

$3.6N_2$:$1H_2$ laminar (single shot)

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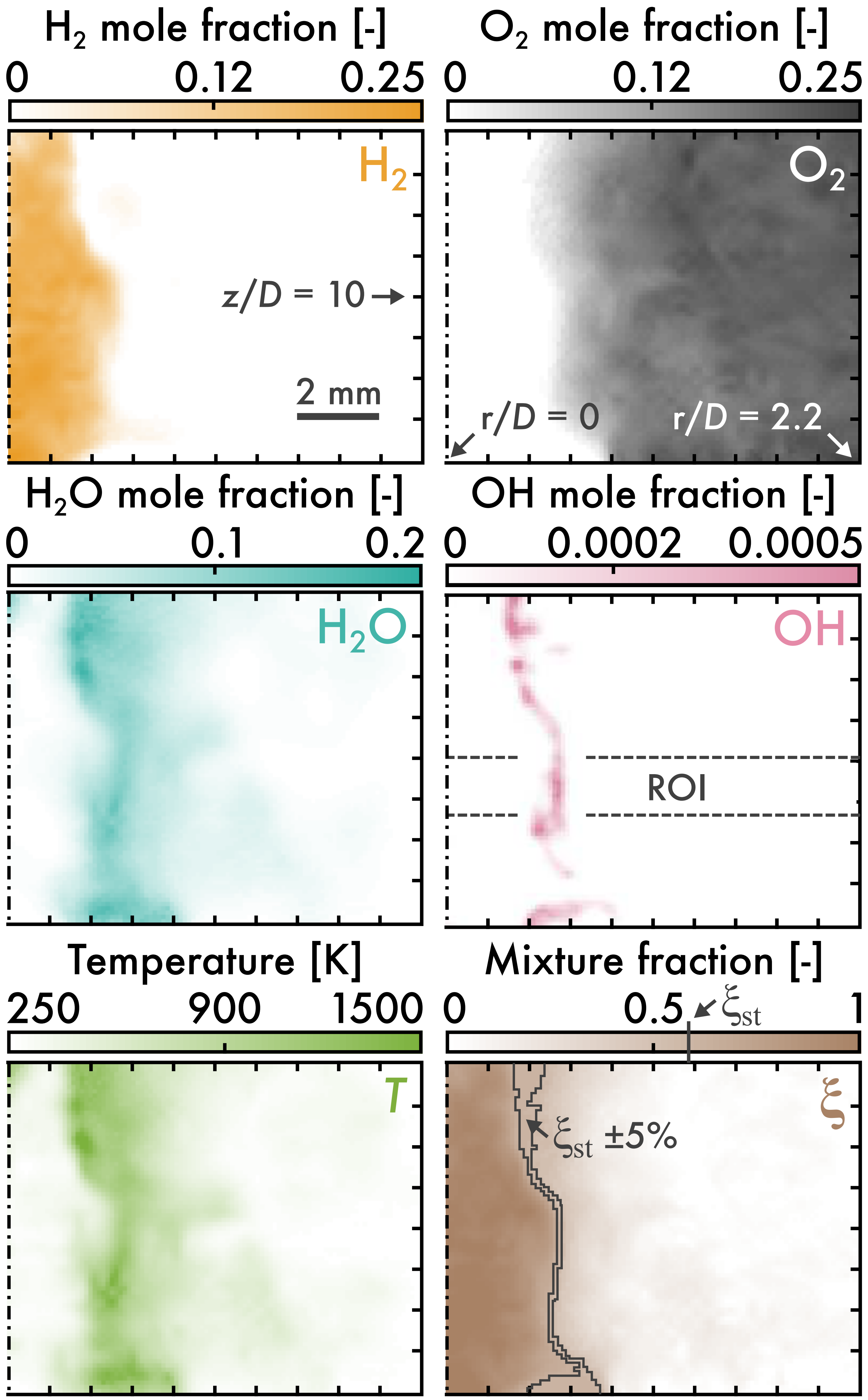
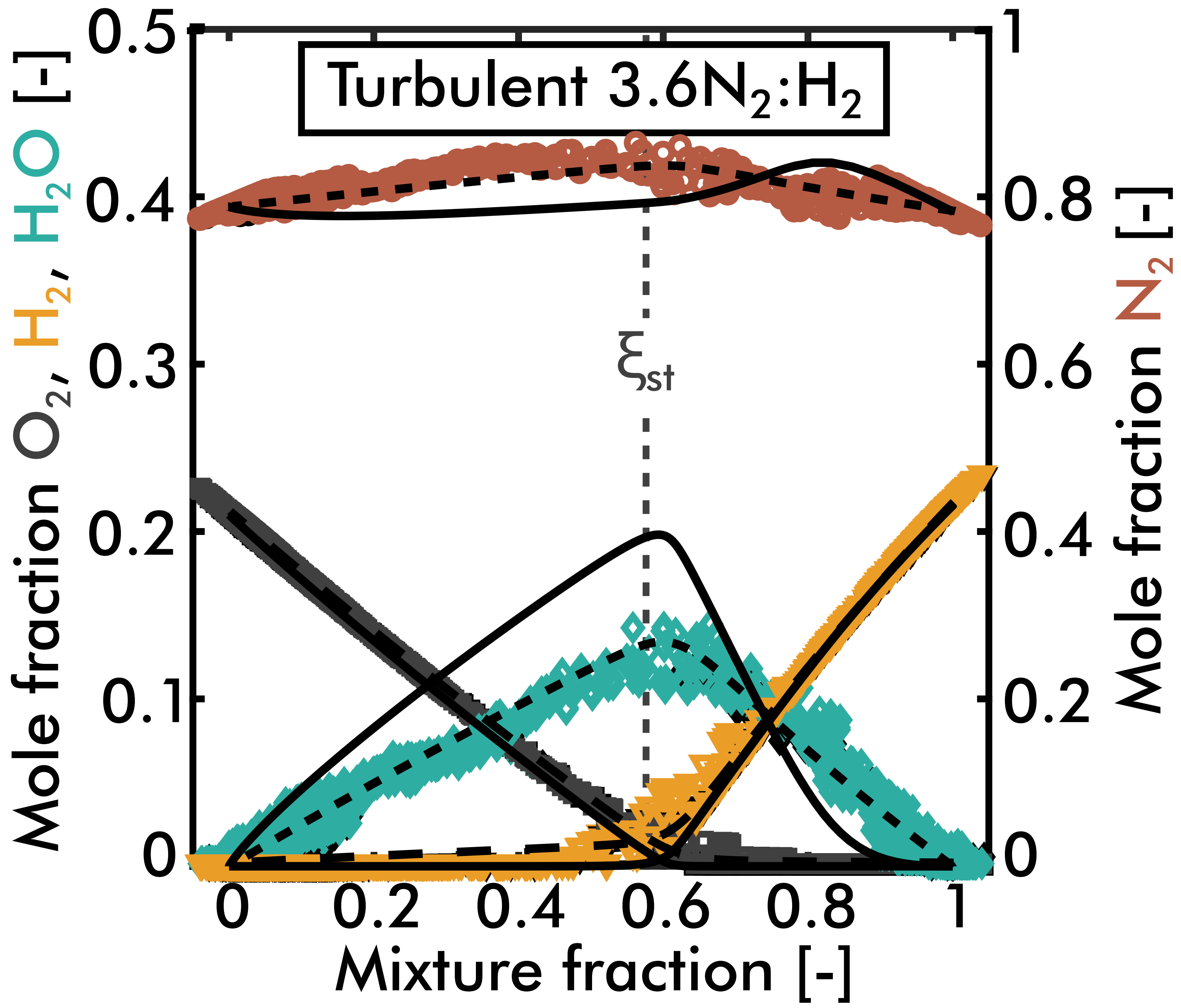
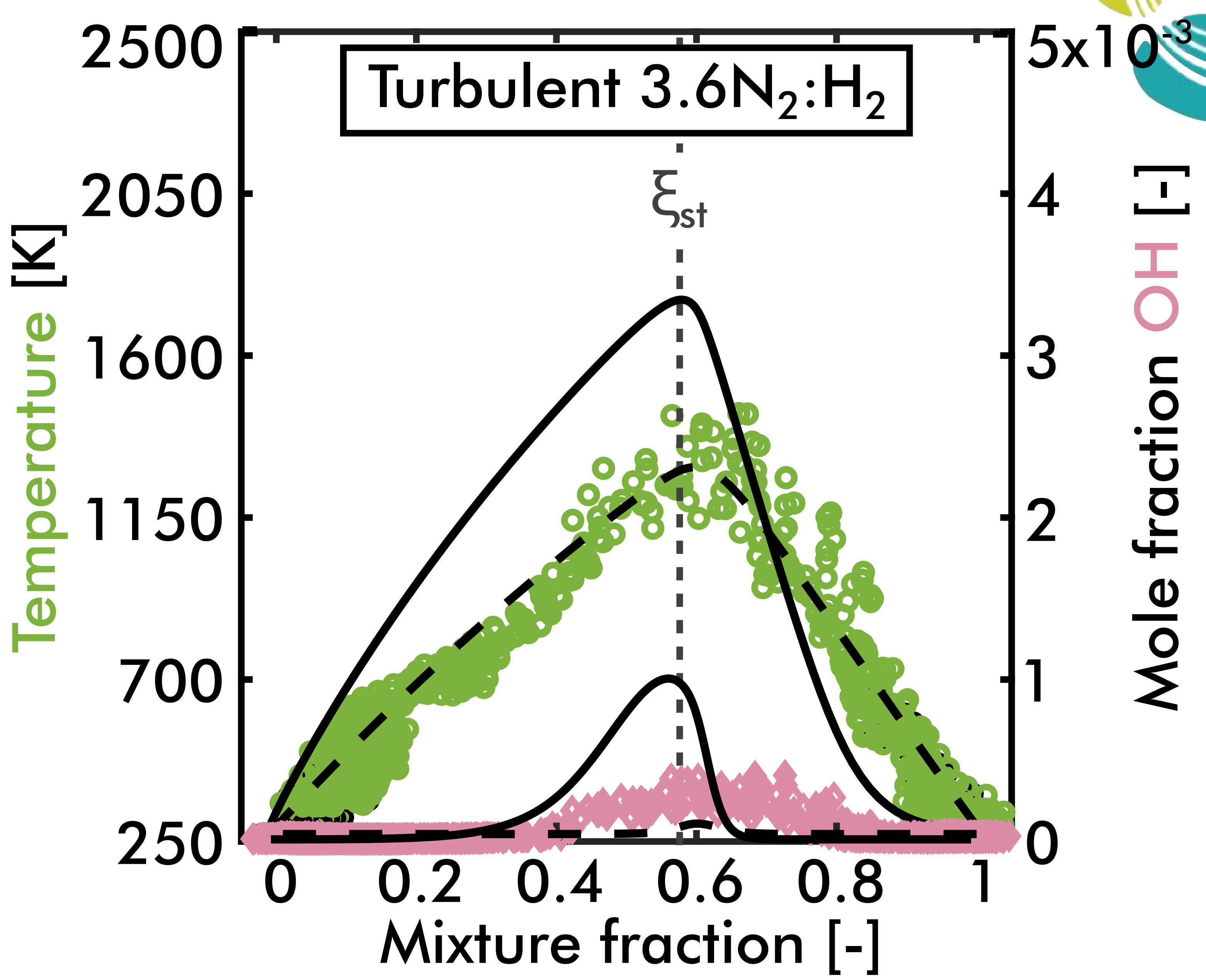
Multi-species 2-D Raman







Multicomponent transport simulations (—) do not capture experiment in turbulent flames but **Le = 1** simulations (- -) do

- Turbulence smears differential diffusion

This lends confidence in this imaging technique

$3.6N_2$:$1H_2$ turbulent (Re = 29,000) (single shot)

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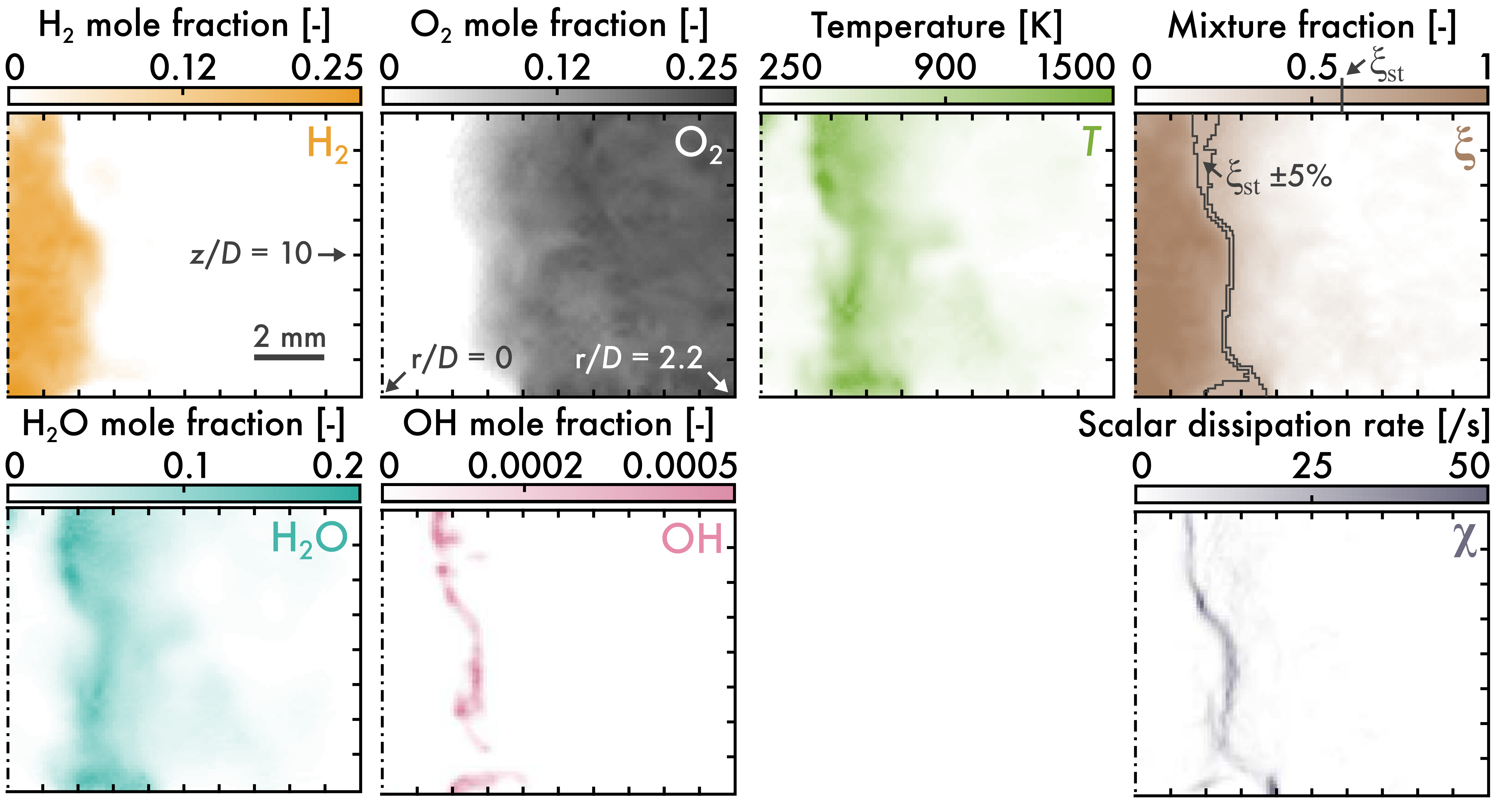
Multi-species 2-D Raman

Why is 2-D desired?

Scalar dissipation rate

$$\chi = 2D\,(\nabla \xi)^2$$



Speed/cost

Compared to 0-D/1-D, data are collected more rapidly in 2-D

This could be very important for "expensive" or "short" experiments

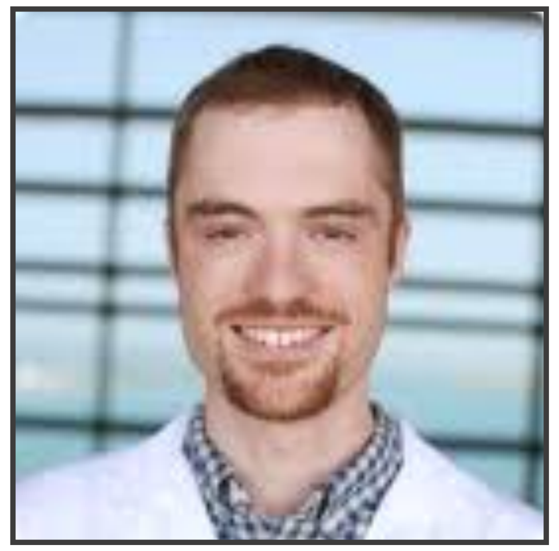
Guiberti et al. Proc. Combust. Inst. 2021(38)

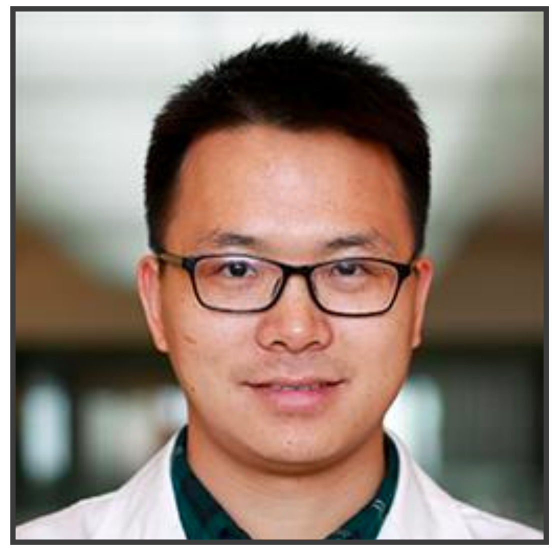
The high-pressure team


Cristian Avila


Abdulrahman Alkhateeb


Hao Tang


Francesco Di Sabatino


Xuren Zhu


Guoqing Wang


Yedhu Krishna


Wesley Boyette


Chaobo Yang


Deanna Lacoste


William Roberts


Gaetano Magnotti


Thibault Guiberti

The University of Sydney


Assaad Masri

IMFT


Sylvain Marragou


Laurent Selle


Thierry Poinsot


Thierry Schuller

H_2 week in Toulouse, February 26th-29th 2024

Questions?