ERCOFTAC Autumn Festival 2025
and
20th Da Vinci Competition 2025

Review Talk

Understanding Jet Flame Structures in Turbulent NH_3/H_2 Combustion

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Acknowledgments

RSM


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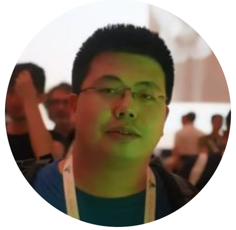
Xun Li

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Bundesministerium für Wirtschaft und Klimaschutz
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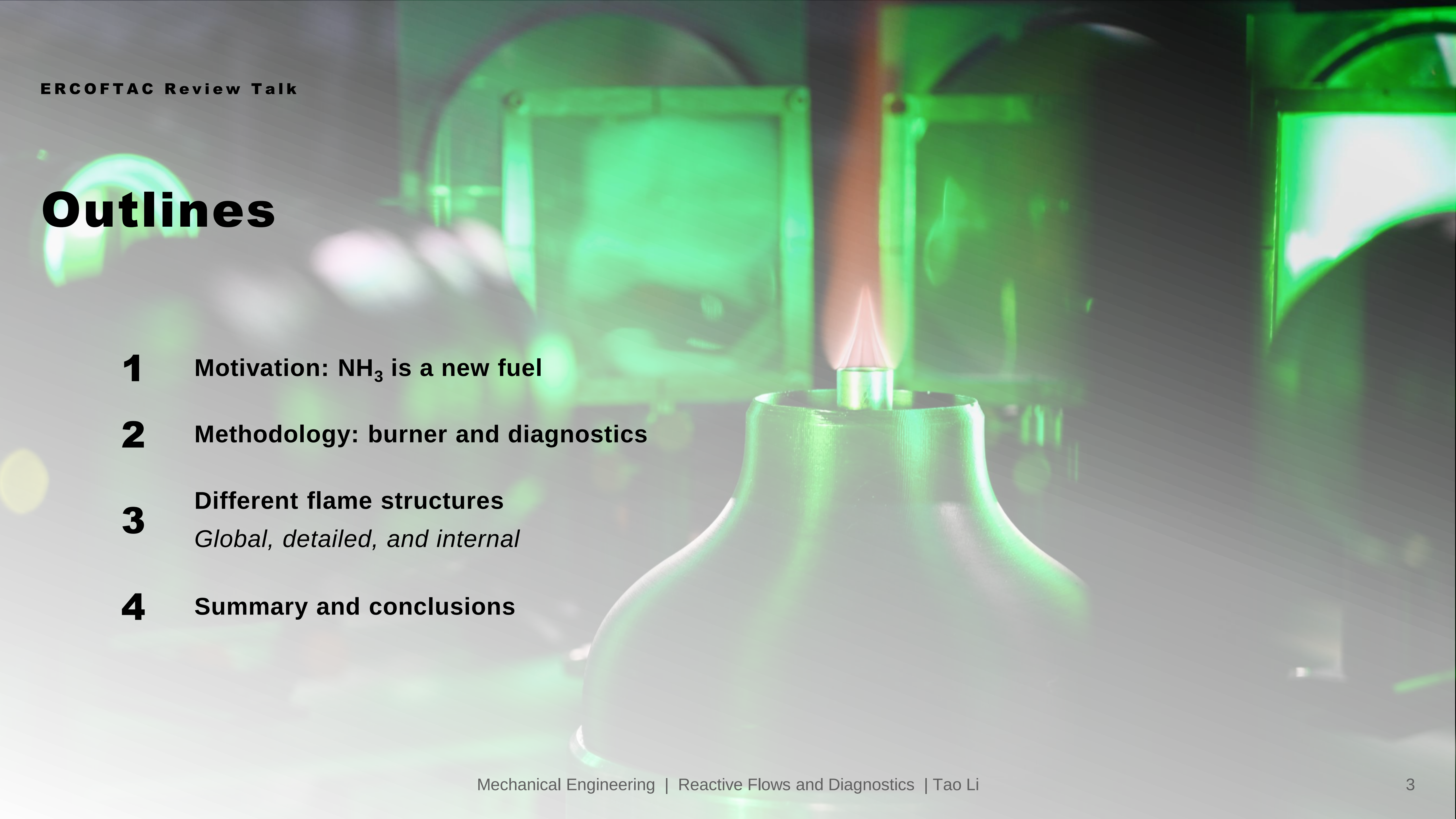
Outlines



1 **Motivation: NH_3 is a new fuel**

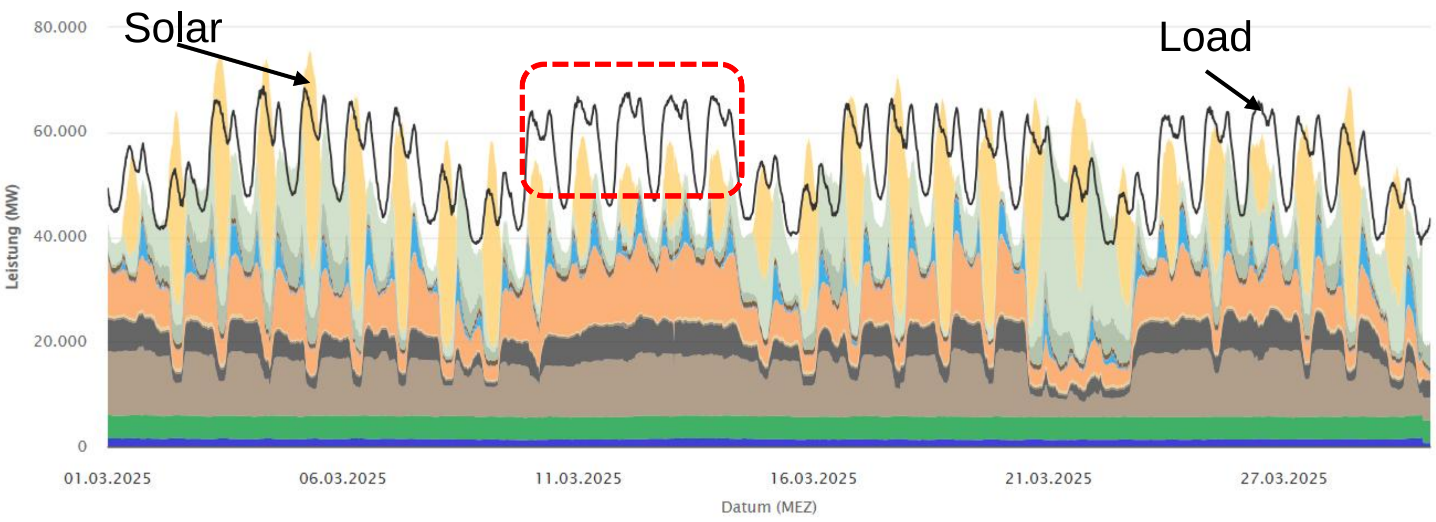
2 **Methodology: burner and diagnostics**

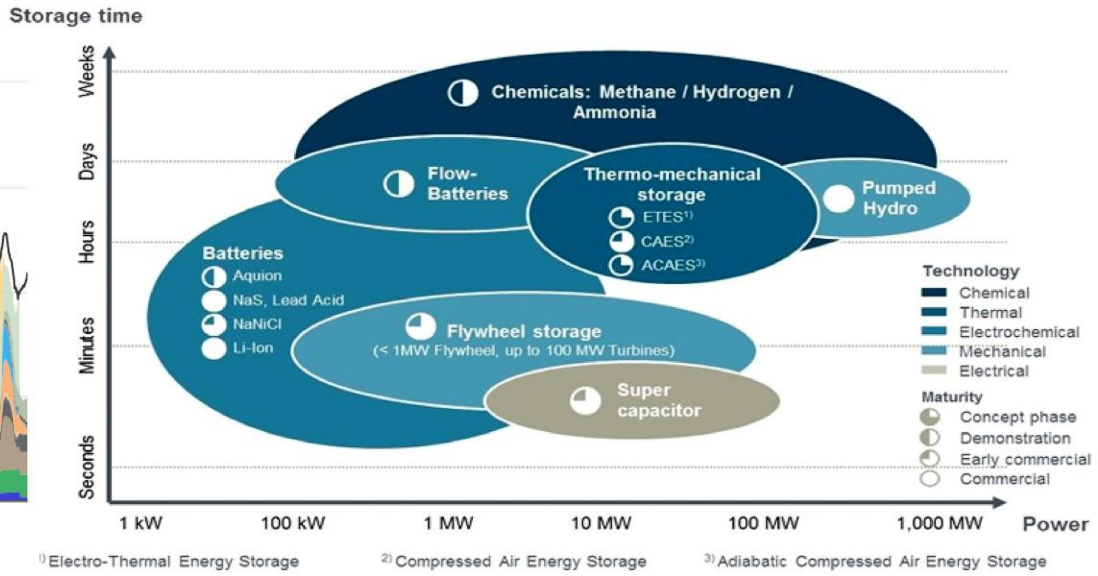
3 **Different flame structures**
Global, detailed, and internal

4 **Summary and conclusions**

Renewable Energy

Germany Electricity Chart, March 2025



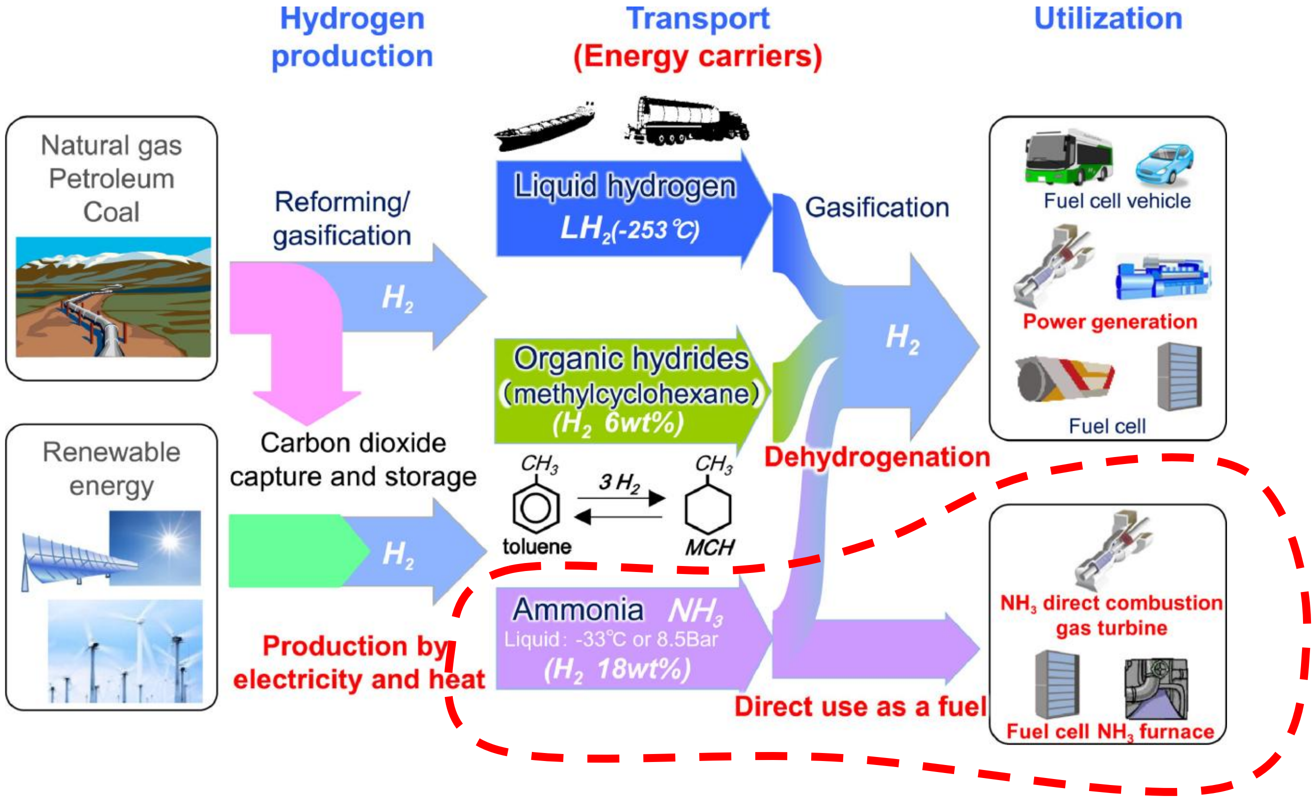


- ► **Electricity consumption dynamics vs. Renewable intermittency**
- ► **Chemicals for long-term & flexible energy storage**

[1] Energy-Charts, Fraunhofer ISE, Germany

[2] **A. Valera-Medina** et al. *Prog. Energy Combust. Sci.* 69 (2018) 63-102

Ammonia Fuel – High Potential



[3] **H. Kobayashi** et al. *Proc. Combust. Inst.* 37(1) (2019) 109-133

Ammonia compared to hydrogen

- High volumetric energy density
- Low storage pressure
- Feasible transportation

What about cost?

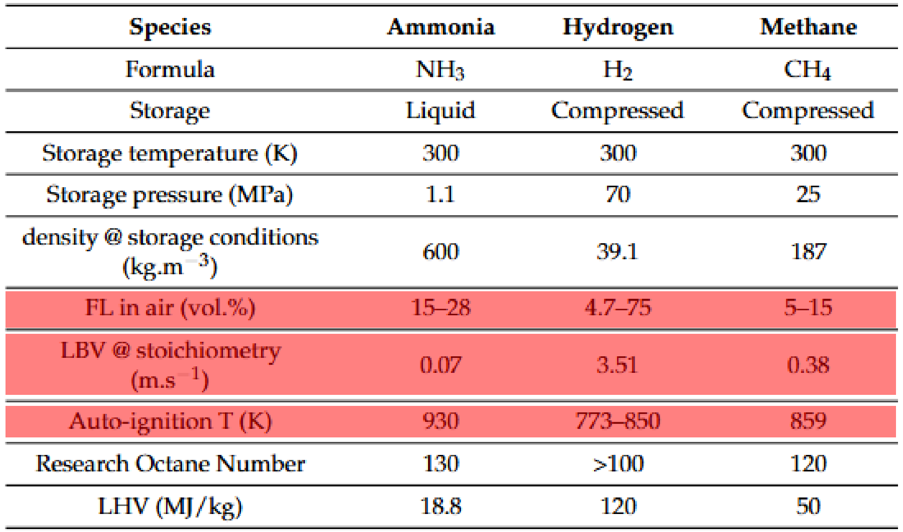
Table 1. Relative Properties and Costs of Ammonia Compared with Liquid Fossil Fuels

Fuel	P (Bar)	Density (kg m^{-3}) (15°C)	LHV (kWh kg^{-1}) (25°C)	LHV (MWh m^{-3}) (25°C)	Cost (USD kg^{-1})	Cost (USD kWh^{-1})
Ammonia	10	603	5.18	3.12	0.30	0.058
Diesel	1	846	12.1	10.2	1.00 (USA)	0.083
LPG	14	388	12.6	4.89	1.00 (Germany)	0.079
Gasoline	1	736	12.1	8.87	1.81 (Japan)	0.15
Bunker Fuel	1	980	10.8	10.6	0.59 (Global average)	0.055

[4] **D. R. MacFarlane** et al. *Joule.* 4(6) (2020) 1186-1205

Ammonia Fuel - Challenges

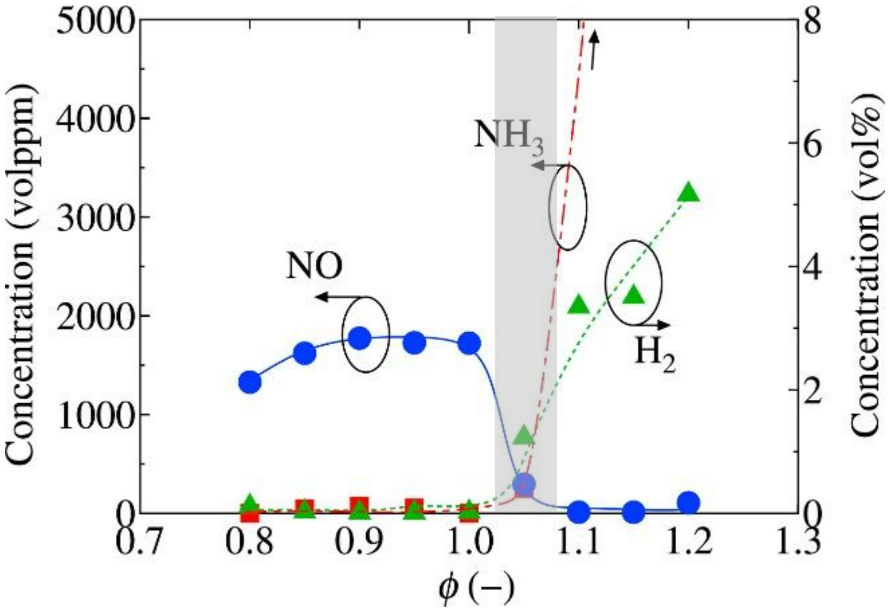
Low chemical reactivity



Species	Ammonia	Hydrogen	Methane
Formula	NH_3	H_2	CH_4
Storage	Liquid	Compressed	Compressed
Storage temperature (K)	300	300	300
Storage pressure (MPa)	1.1	70	25
density @ storage conditions ($kg.m^{-3}$)	600	39.1	187
FL in air (vol.%)	15–28	4.7–75	5–15
LBV @ stoichiometry ($m.s^{-1}$)	0.07	3.51	0.38
Auto-ignition T (K)	930	773–850	859
Research Octane Number	130	>100	120
LHV (MJ/kg)	18.8	120	50

Narrow flammable limits, low burning speed, high ignition temperature

Emissions



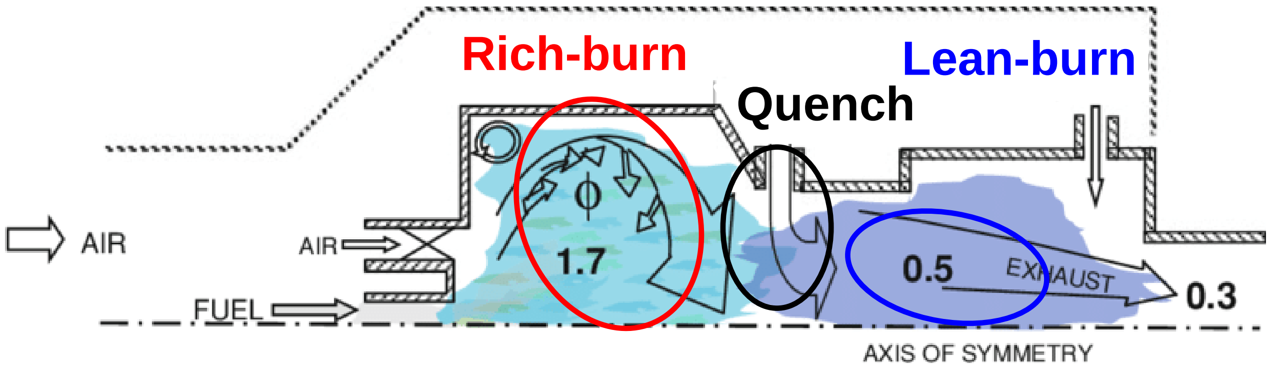
Solution: partial cracking / fuel blending

Solution: staged combustion

[5] **C. Mounaïm-Rousselle** et al. *Energies* 14 (14) (2021) 4141

[6] **X. Zhu** et al. *Energy Fuels* 2024, 38, 1, 43–60

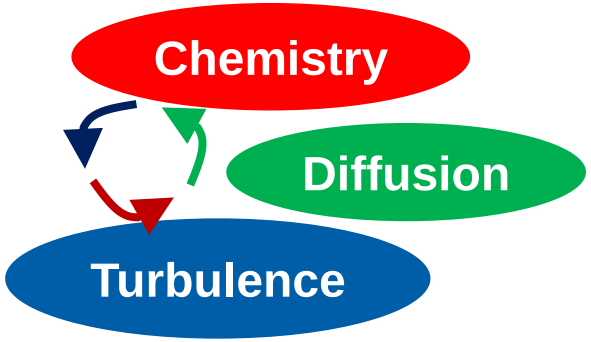
Staged Combustion



- Staged combustion systems (RQL) show promising performance[7,8]
- Challenges in **flame stabilization and reducing NO_x** due to complex chemistry-turbulence interaction, multi-regime reaction, and diffusion[9,10]

Approaches

- Lab-scale burners, experiments
- Well-defined boundary conditions
- In-situ laser diagnostics
- Coupling with simulations



A better understanding of turbulent flame structures

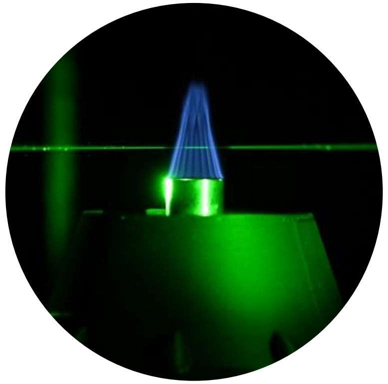
[7] **E. Okafor** et al. *Proc. Combust. Inst.* 37 (4) (2019), pp. 4597–4606
[8] **G. S. Samuelsen** et al. *Heat Mass Transfer* 49, (2013) 219–231
[9] **A. Stagni** et al. *J. Chem. Eng.* 471 (2023) 144577
[10] **A. Hayakawa** et al. *Int. J. Hydrogen Energy* 42 (19) (2017), pp. 14010–14018

Research Approaches

- From laminar to turbulent flow
- From simple to complex geometry
- From atmospheric to pressurized condition
- Isolate subprocesses and interactions

- Different fuels: H_2, NH_3, blends
- Academic and industrial collaboration
- **Phenomenological understanding + validation data**

Laminar Flame

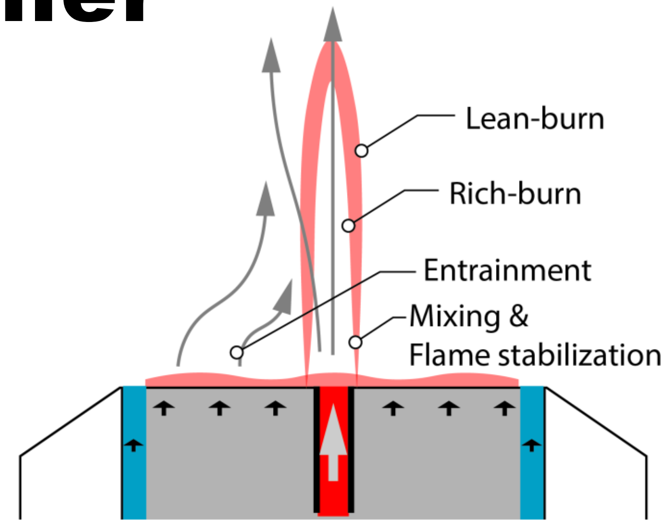


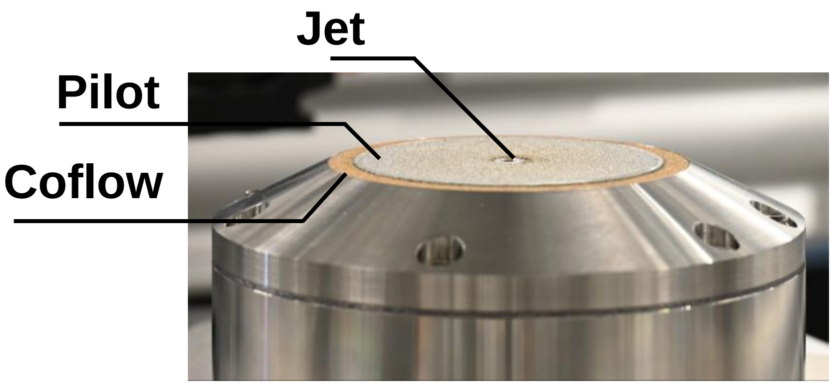
Turbulent Jet Flame

Multi-Regime Flame

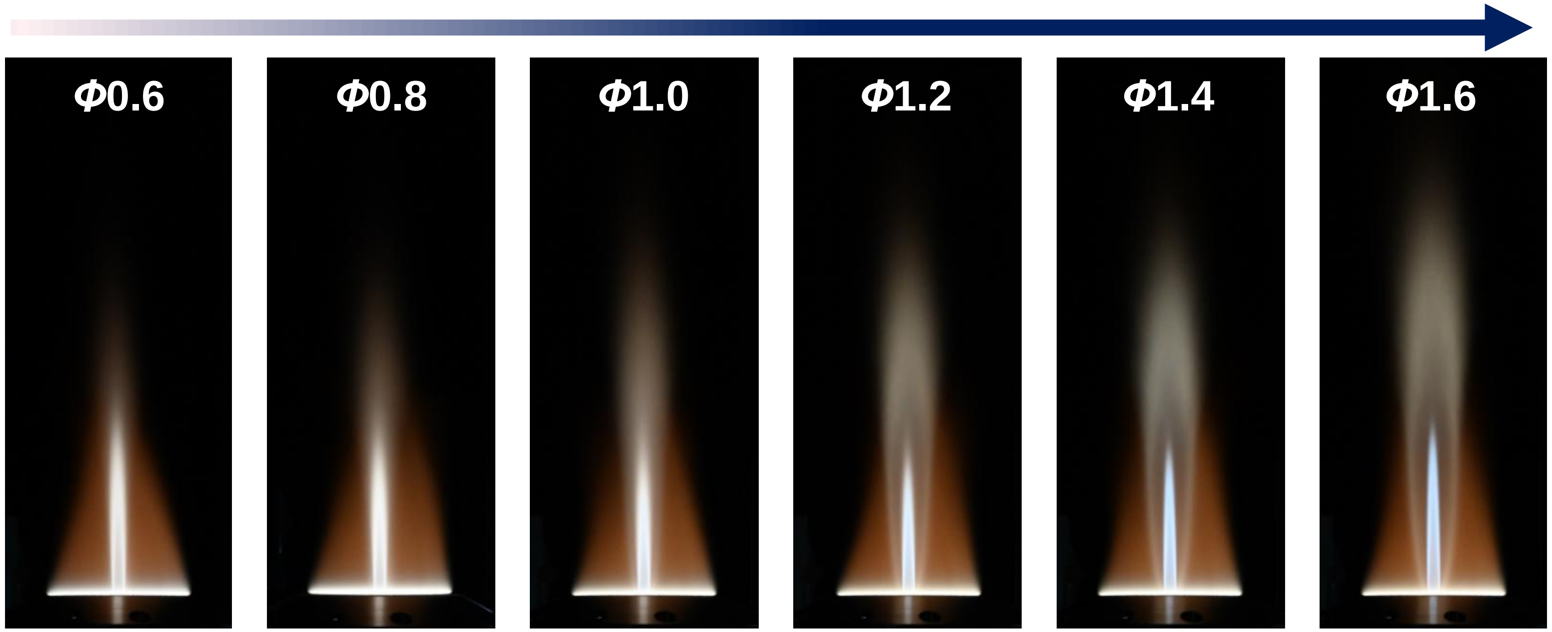
Flame under Pressure

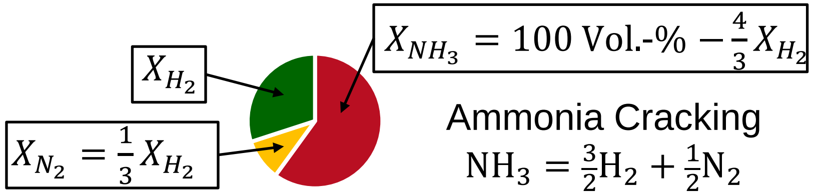
Burner





Stratification: increasing jet fuel





X_{H_2}

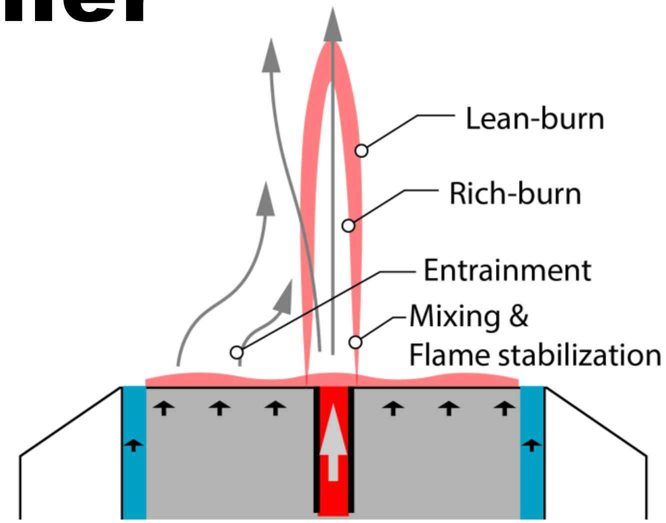
$X_{N_2} = \frac{1}{3} X_{H_2}$

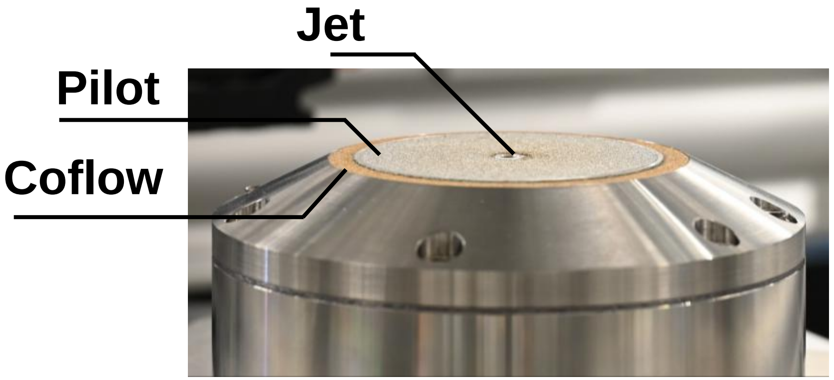
$X_{NH_3} = 100 \text{ Vol.-\%} - \frac{4}{3} X_{H_2}$

Ammonia Cracking

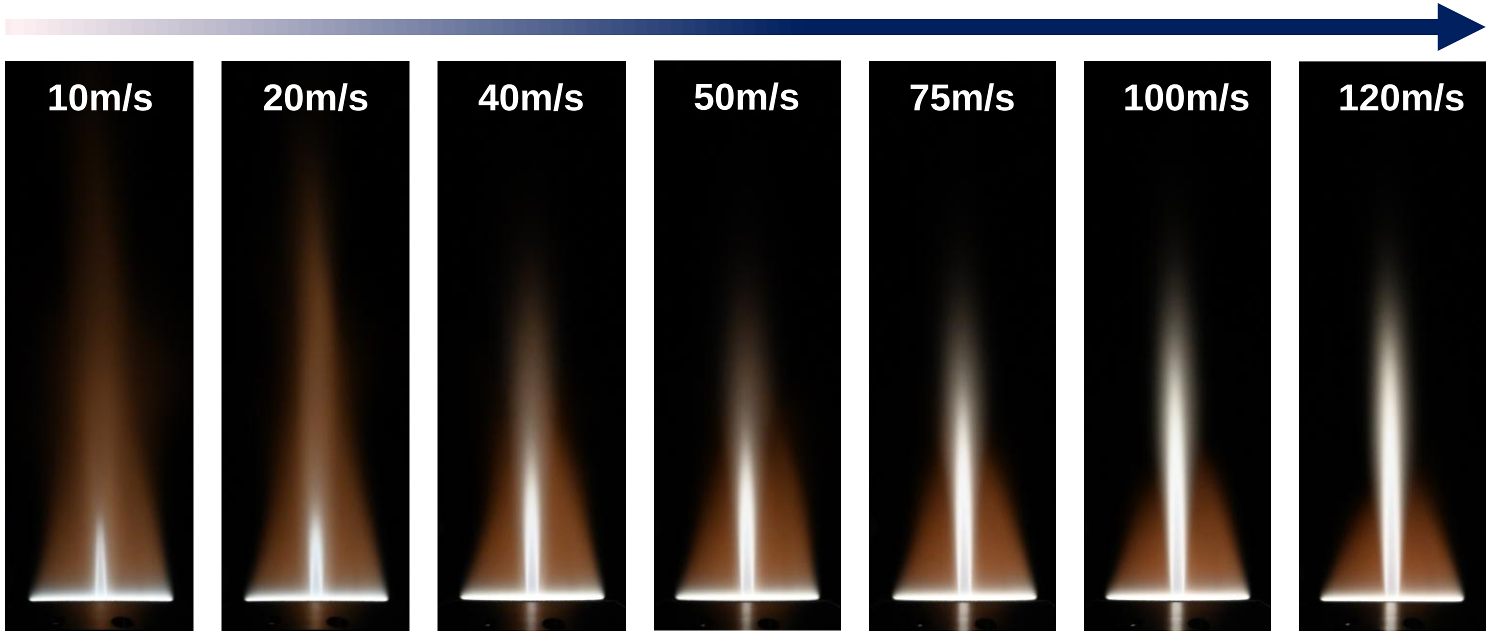
$\mathrm{NH_3} = \frac{3}{2}\mathrm{H_2} + \frac{1}{2}\mathrm{N_2}$

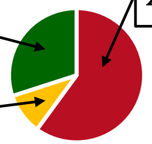
Burner





Turbulence: increasing jet velocity





X_{H_2}

$X_{N_2} = \frac{1}{3} X_{H_2}$

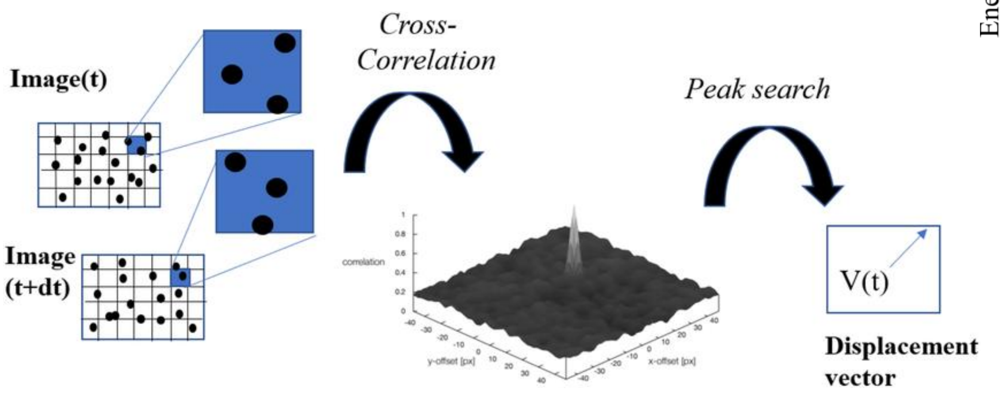
$X_{NH_3} = 100 \text{ Vol.-\%} - \frac{4}{3} X_{H_2}$

Ammonia Cracking

$NH_3 = \frac{3}{2}H_2 + \frac{1}{2}N_2$

Which Laser Diagnostics?

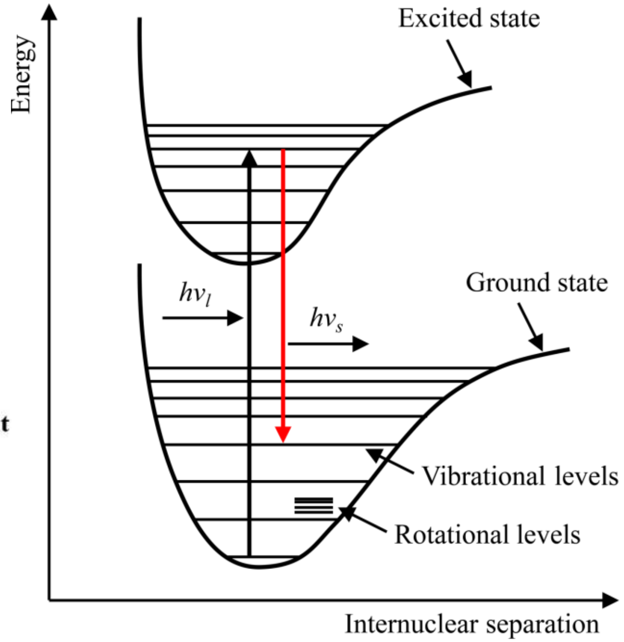
Particle image velocimetry



[22] **A. Giannopoulos** et al. *Exp Fluids* 63, 57 (2022)

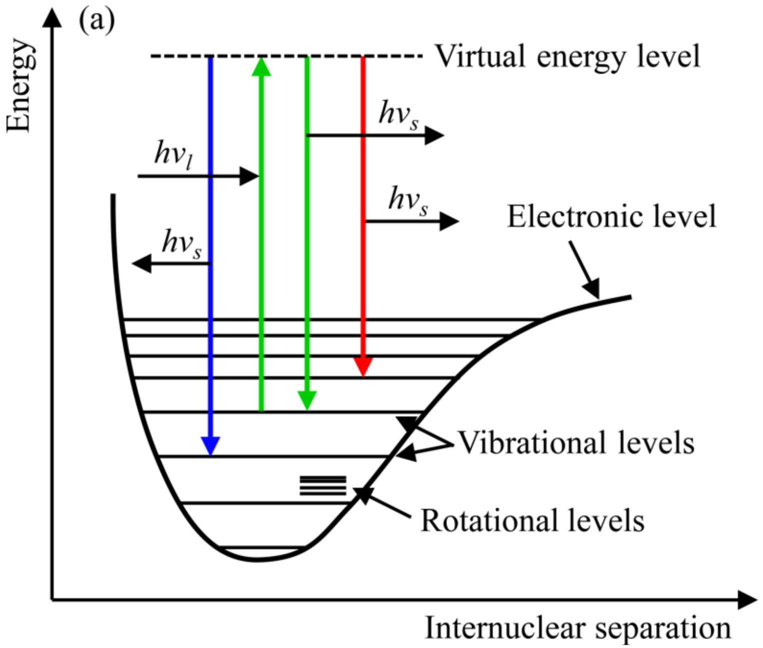
Flow velocity fields

Laser-induced fluorescence



Flame topology, intermediates

Raman/Rayleigh scattering



Rayleigh

Density/
Temperature

Stokes Raman

Species
concentration

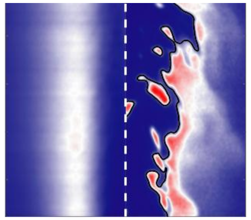
What Do I Mean by ‘Flame Structure’?

Global Structures

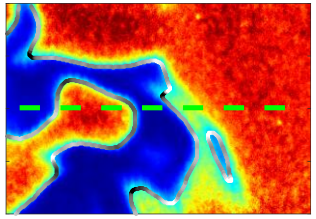
= *macroscopic*

- Flame front
- Curvature
- Surface area, burning speed

OH-LIF



Rayleigh Temperature



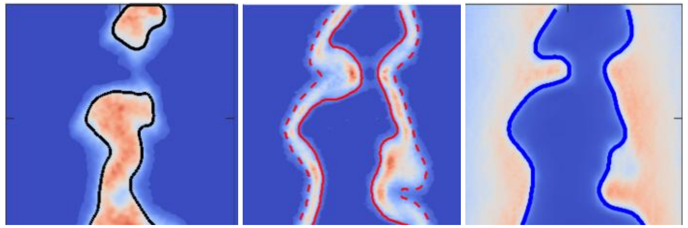
Examples in literature:

[11] **O. Chaib** et al. *Proc. Combust. Inst.* 40 (1-4) (2024), 105763
[12] **X. Cai** et al. *Proc. Combust. Inst.* 39 (1-4) (2023), 4215-4226
[13] **X. Wei** et al. *Combust. Flame* 249 (2023) 112600

Detailed Structures

- Reaction zone
- Scalars, intermediates
- **Qualitative** distribution

NH_3-LIF NH-LIF OH-LIF



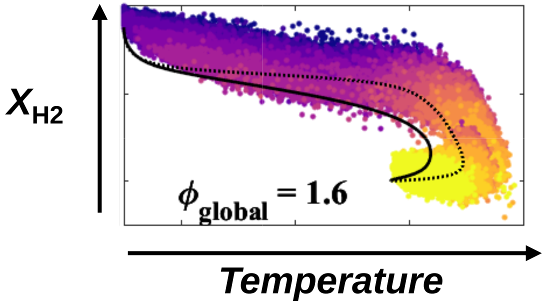
Examples in literature:

[14] **C. Brackmann** et al. *Combust. Flame* 163 (2016) 370-381
[15] **Q. Fan et al.** *Combust. Flame* 238 (2022) 111943
[16] **G. Wang** et al. *Fuel* 367 (2024), 131430
[17] **H. Dai** et al. *Combust. Flame* 274 (2025), 114031

Internal Structures

= *microscopic*

- Temperature
- Concentration of major molecules
- **Quantitative** thermochemistry



Examples in literature:

[18] **R.S. Barlow** et al. *Combust. Flame* 120 (2000) 549-569
[19] **W. Meier** et al. *Combust. Flame* 123 (2000) 326-343
[20] **H. Tang** et al. *Combust. Flame* 237 (2022) 111840
[21] **ARW Macfarlane** et al. *Combust. Flame* 279 (2025) 114388

Increasing level of detail, but higher complexity in experiments!

Leading Scientific Questions

Global

Q1: What are the **flame topology characteristics** of the premixed ammonia jet flames, and how are they influenced by turbulence?

Detailed

Q2: How can we visualize the **reaction zone containing multiple species**, and how are they modified by differential diffusion and turbulence?

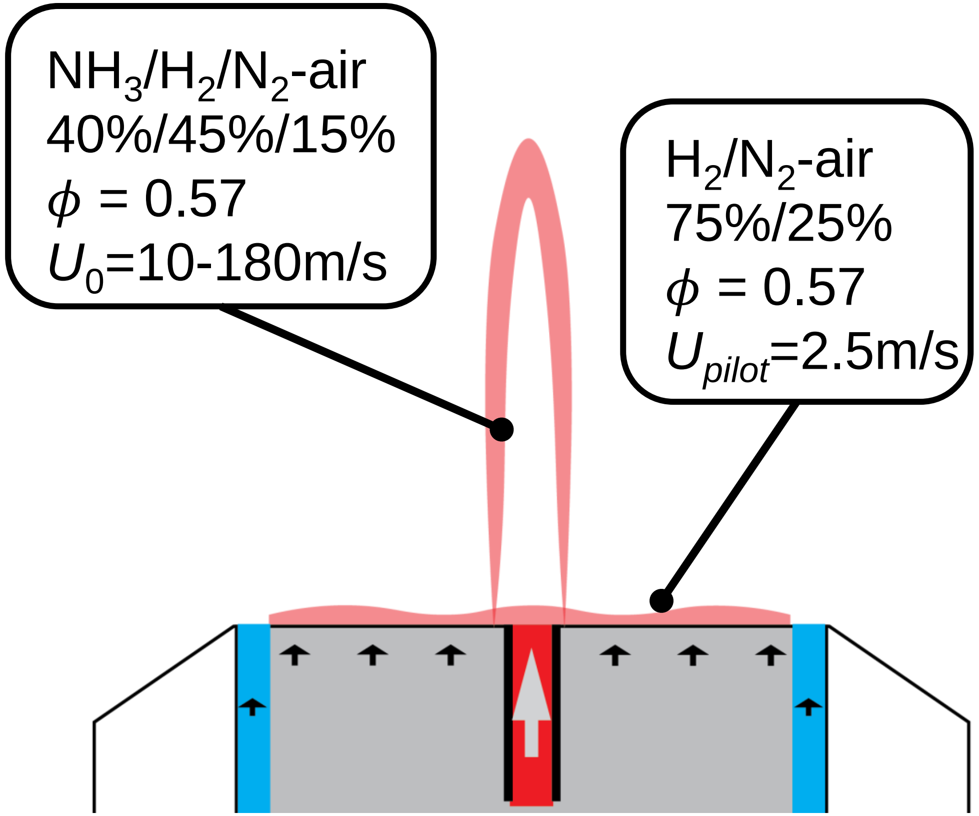
Internal

Q3: How to quantify the **thermochemical states** of stratified flames, and what can we learn from the data?

Q1: What are the **flame topology characteristics** of the premixed ammonia jet flames, and how are they influenced by turbulence?

Lean Premixed Jet Flame

High-*Ka*, fully premixed
(same H/N/O ratio)



$NH_3/H_2/N_2$-air
40%/45%/15%
ϕ = 0.57
U_0=10-180m/s

H_2/N_2-air
75%/25%
ϕ = 0.57
U_{pilot}=2.5m/s

Karlovitz number[24] :

$$Ka^2 = \left(\frac{U'}{S_\mathrm{L}}\right)^3 \frac{l_\mathrm{F}}{l}$$

S_L: laminar flame speed → simulation
l_F: thermal flame thickness → simulation

S_L = 0.112 m/s, l_F = 1.02 mm

U': turbulent velocity → PIV
l : integral length scale → PIV

l = 4.1-3.1 mm, U'=3.3-31.6 m/s

***Ka* ~ 75-2140**

[23] **T. Li** et al., *Journal of Ammonia Energy*, 3(1) (2024) 37
[24] **N. Peters**, Turbulent Combustion, Cambridge University Press, 2000

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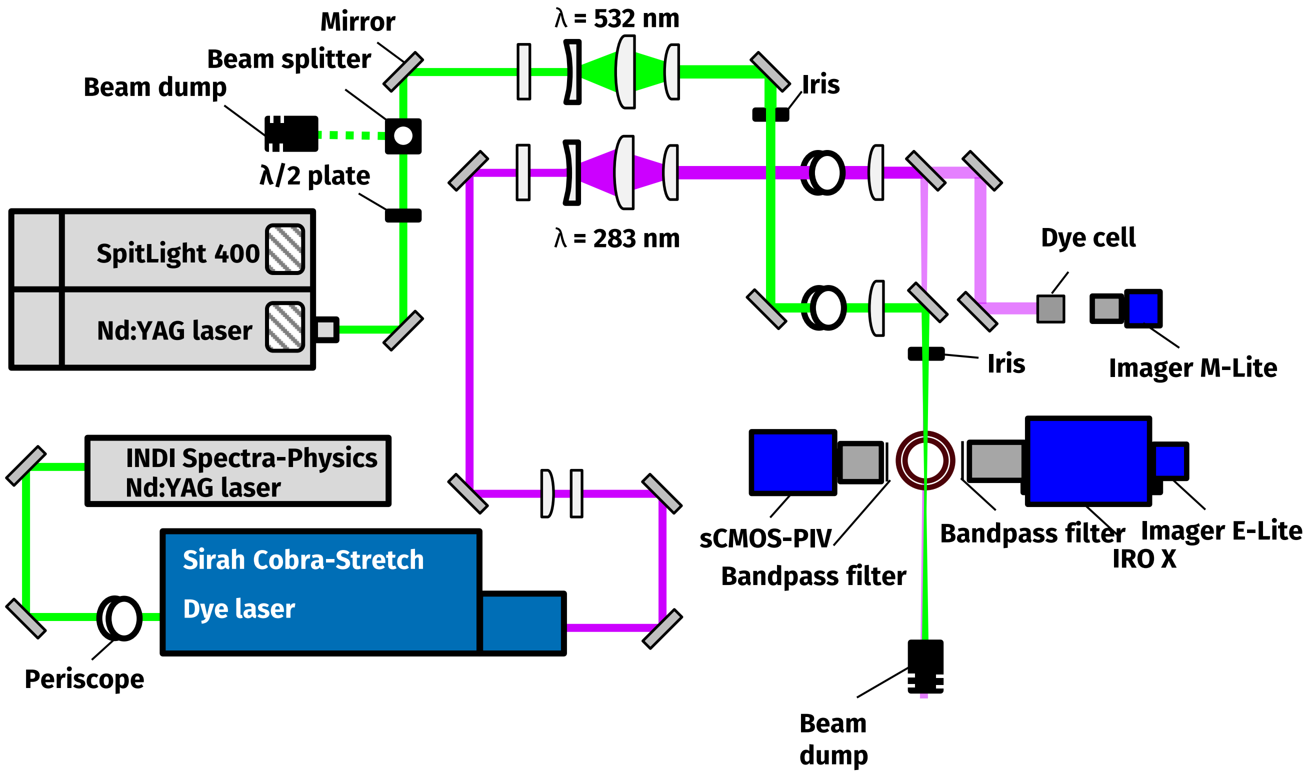
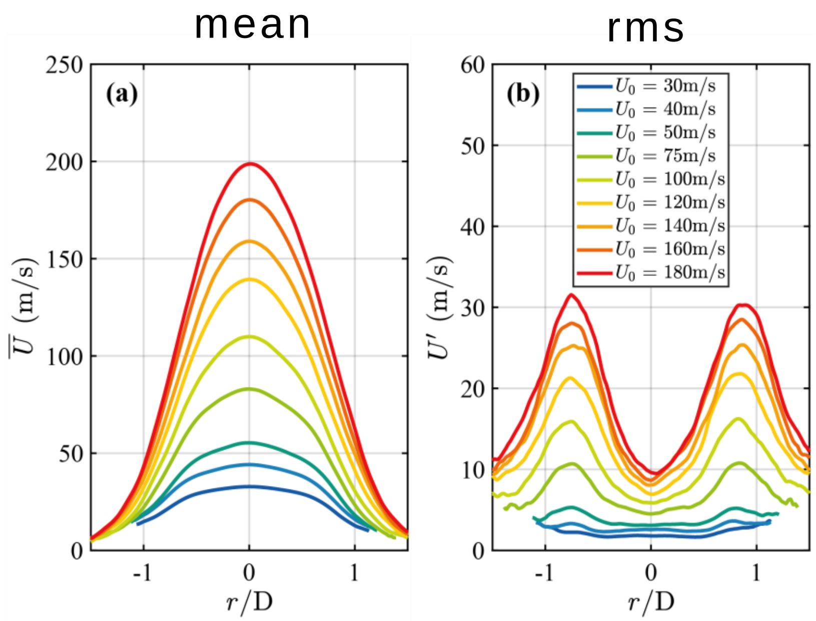
OH-LIF and PIV measurements



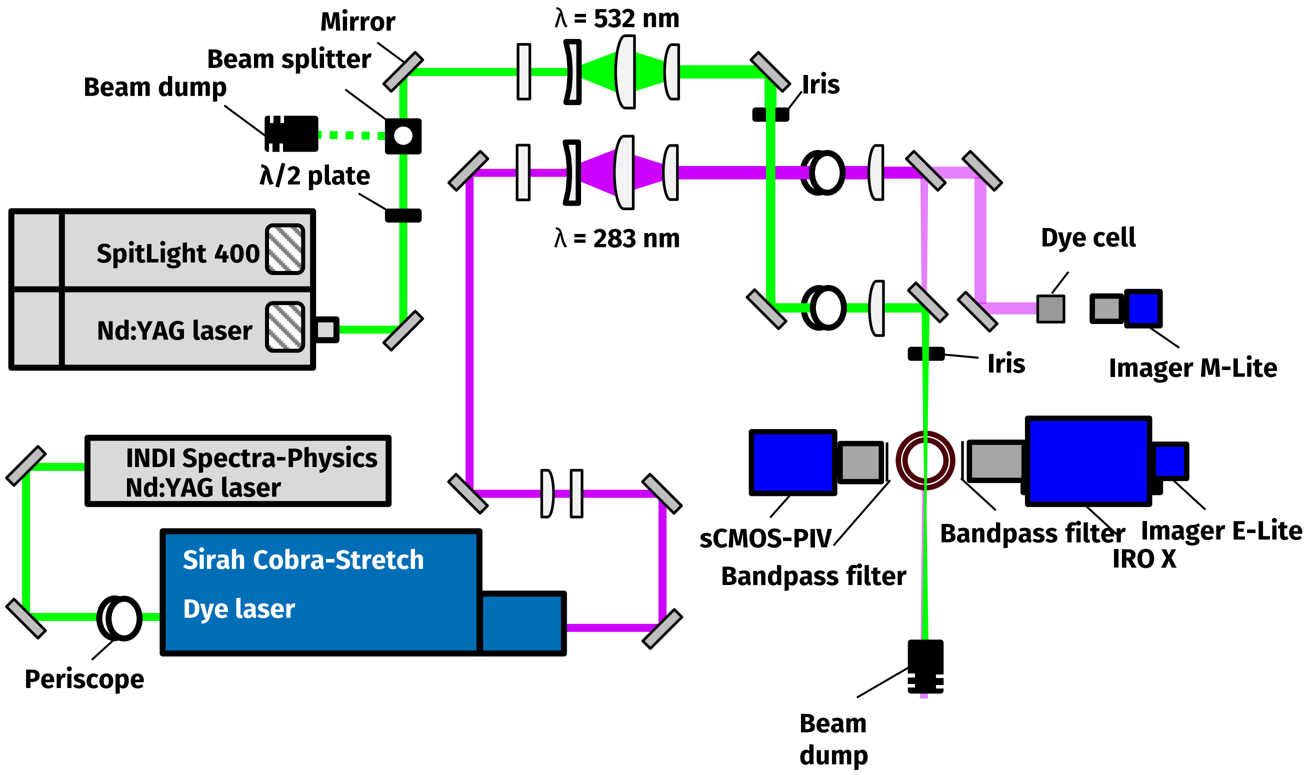
PIV

- Nd:YAG laser λ = 532 nm
- Double pulses Δt=1 μs
- Al_2O_3 flow tracer particles



[25] **T. Li** et al., *Proc. Combust. Inst.* 40 (2024) 105759
[26] **S. Shi** et al., *Proc. Combust. Inst.* 40 (2024) 105225

OH-LIF and PIV measurements



PIV

- Nd:YAG laser *λ* = 532 nm
- Double pulses Δ*t*=1 μs
- Al_2O_3 flow tracer particles

mean

rms

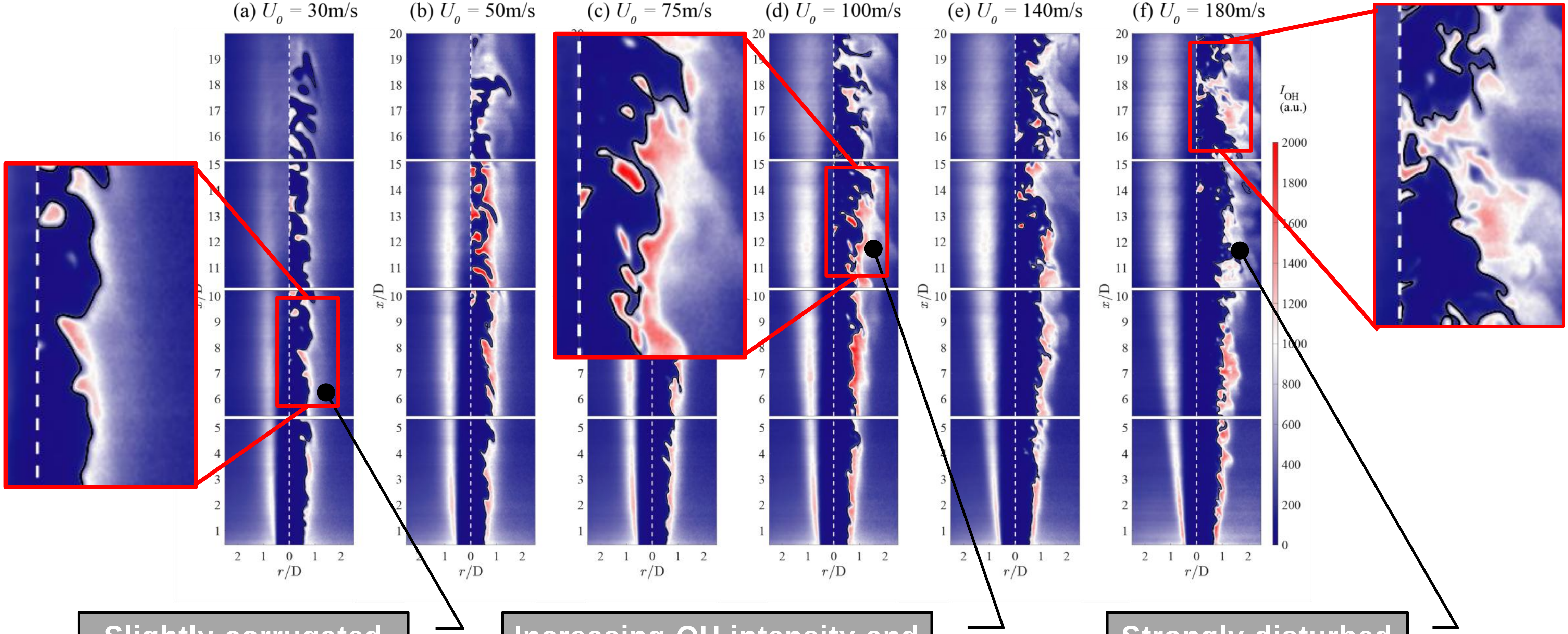
OH-PLIF

- Nd:YAG pumped dye laser
- Excitation at λ ~ 283 nm
- Detection in 310-340 nm
- Spatial resolution: 100 μm

[25] **T. Li** et al., *Proc. Combust. Inst.* 40 (2024) 105759
[26] **S. Shi** et al., *Proc. Combust. Inst.* 40 (2024) 105225

Global Flame Structures

Ka~75 → Increasing U_0 → *Ka*~2140

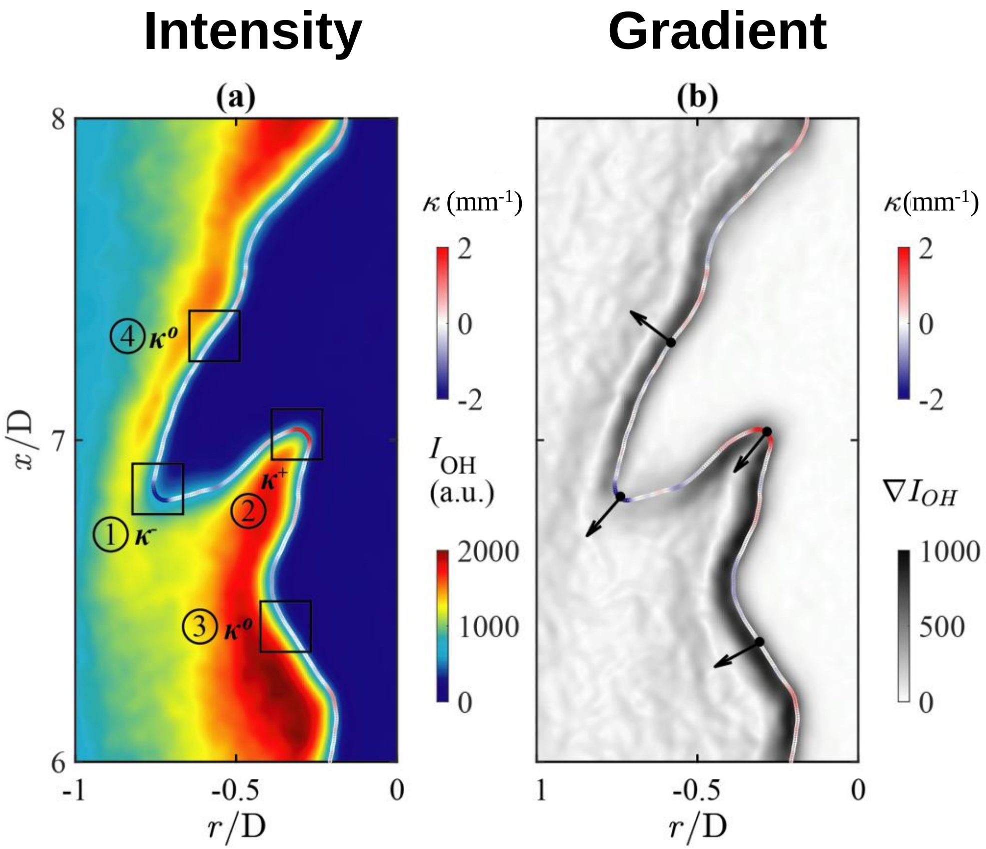


Slightly corrugated flame front

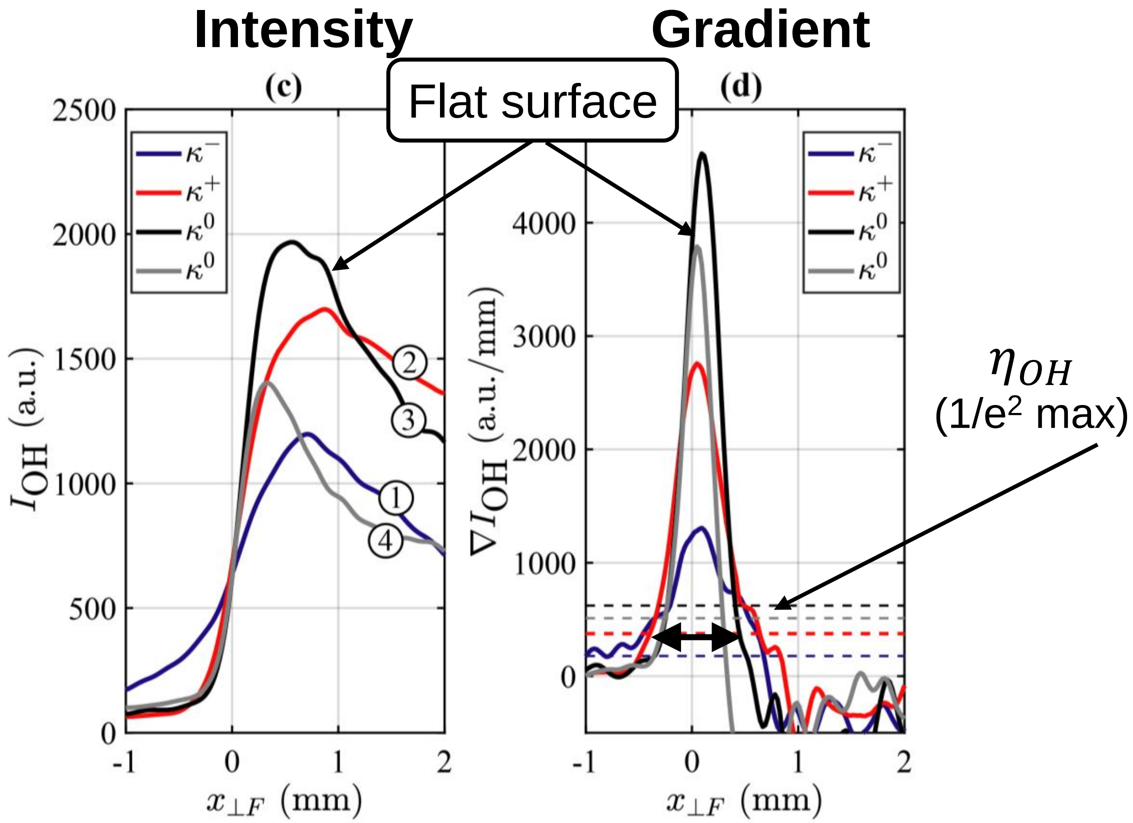
Increasing OH intensity and its gradient

Strongly disturbed flame

OH Intensity and Gradient



Flame coordinates



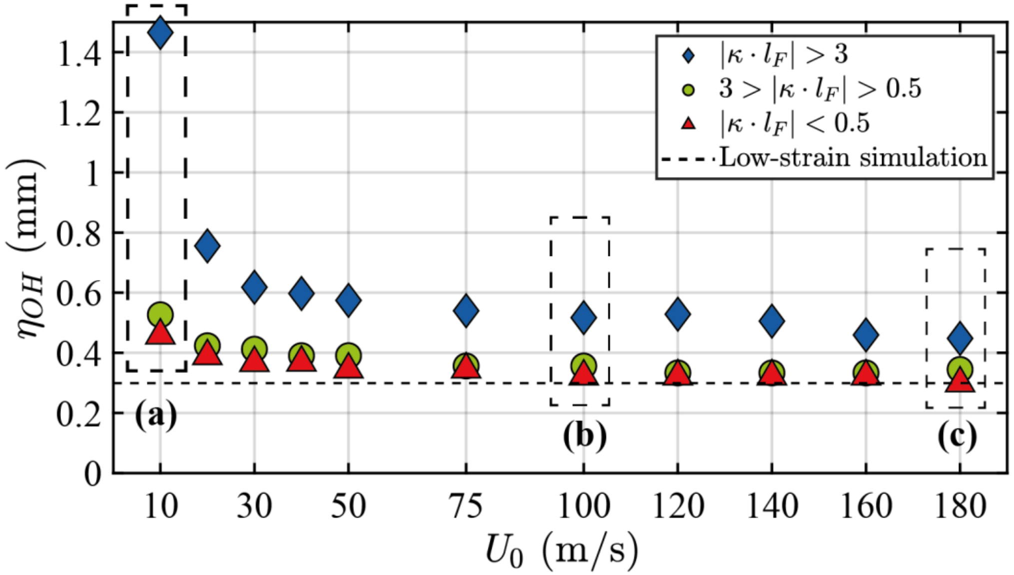
Flat surface

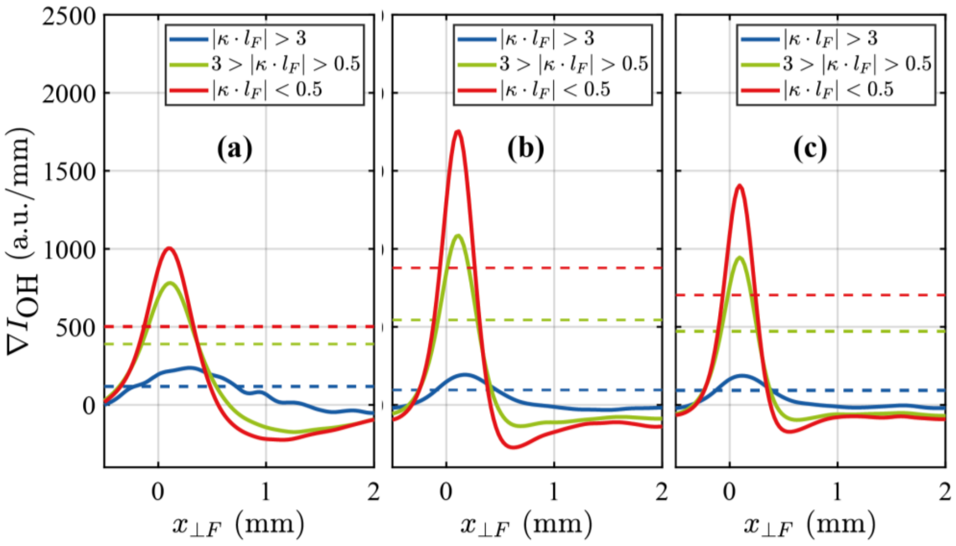
η_{OH}
(1/e^2 max)

- Positively curved surface has higher intensity than negatively curved surface
- Flat surfaces have **the highest** intensity and gradients
- ***What about the OH layer thickness?***

[23] **T. Li** et al., *Journal of Ammonia Energy*, 3(1) (2024) 37

OH layer thickness





Increasing turbulence:

- All thickness reduce due to strain
- Dual role of turbulence: increasing (or decreaing) gradient at low (or high) turbulence

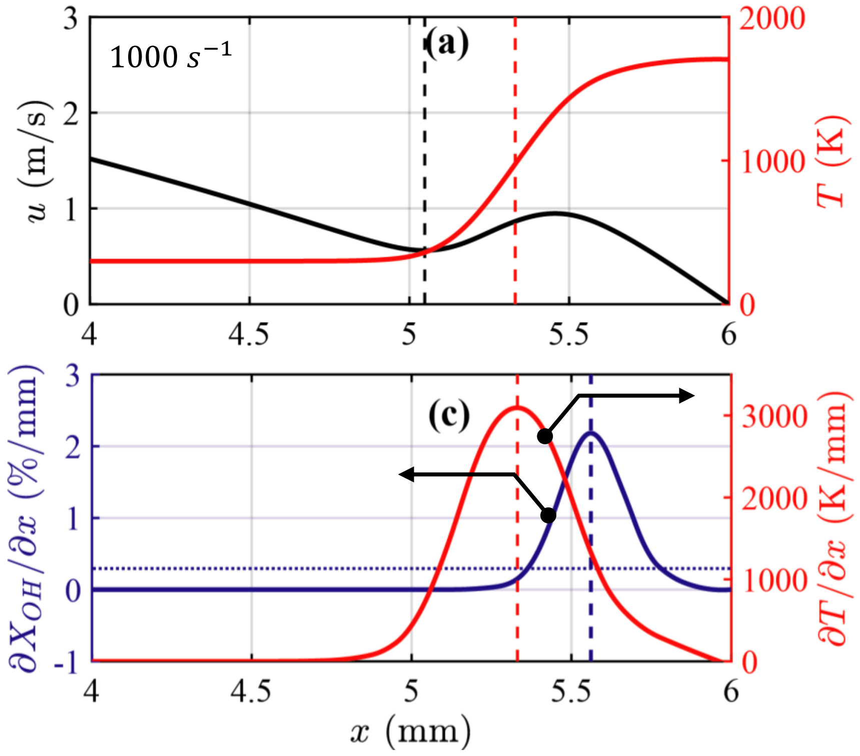
Flat surface:

- OH layer thickness converges towards the laminar value
- No broadening at high *Ka* numbers

- ***Why?***

[23] **T. Li** et al., *Journal of Ammonia Energy*, 3(1) (2024) 37

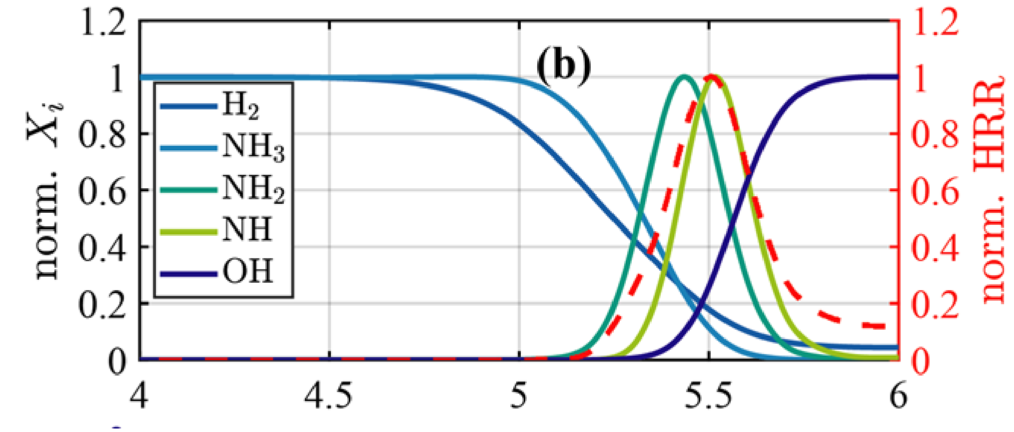
Counter-flow Flame Simulation



Unburned **Burned**

- **OH layer is at high-temperature zone**
- Turbulent eddies may not be able to penetrate into the OH layer even at high turbulence

- However, the reaction zone contains other intermediate species

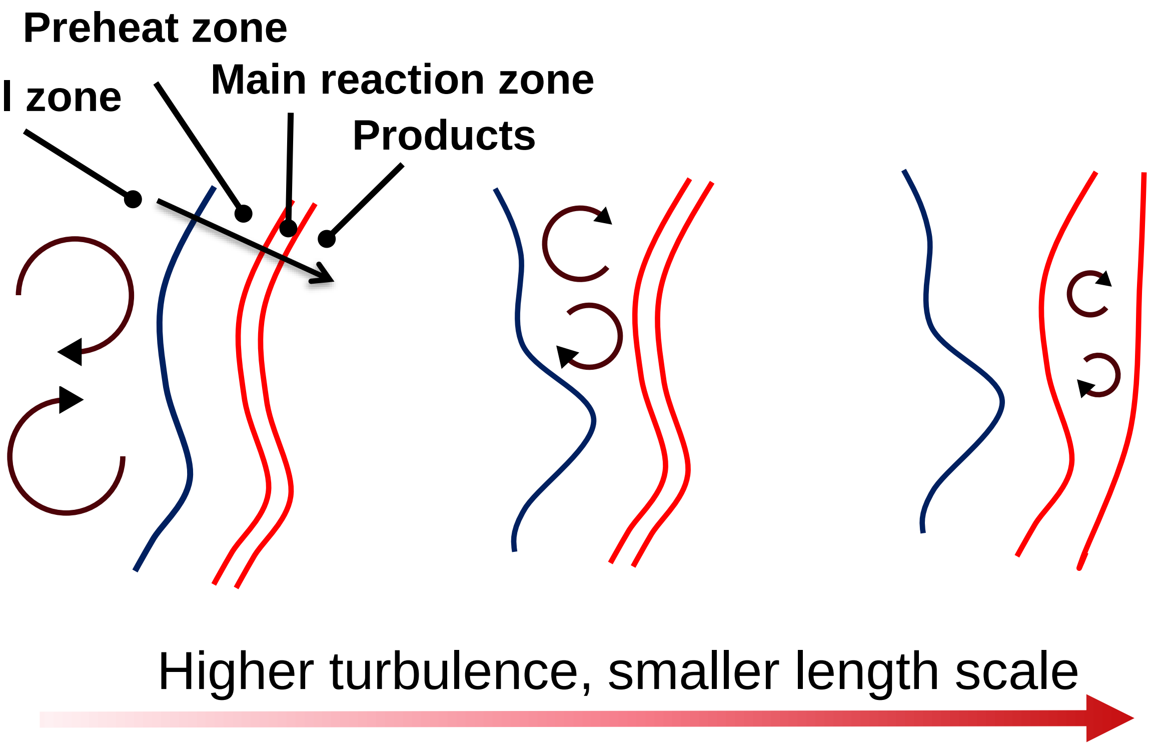


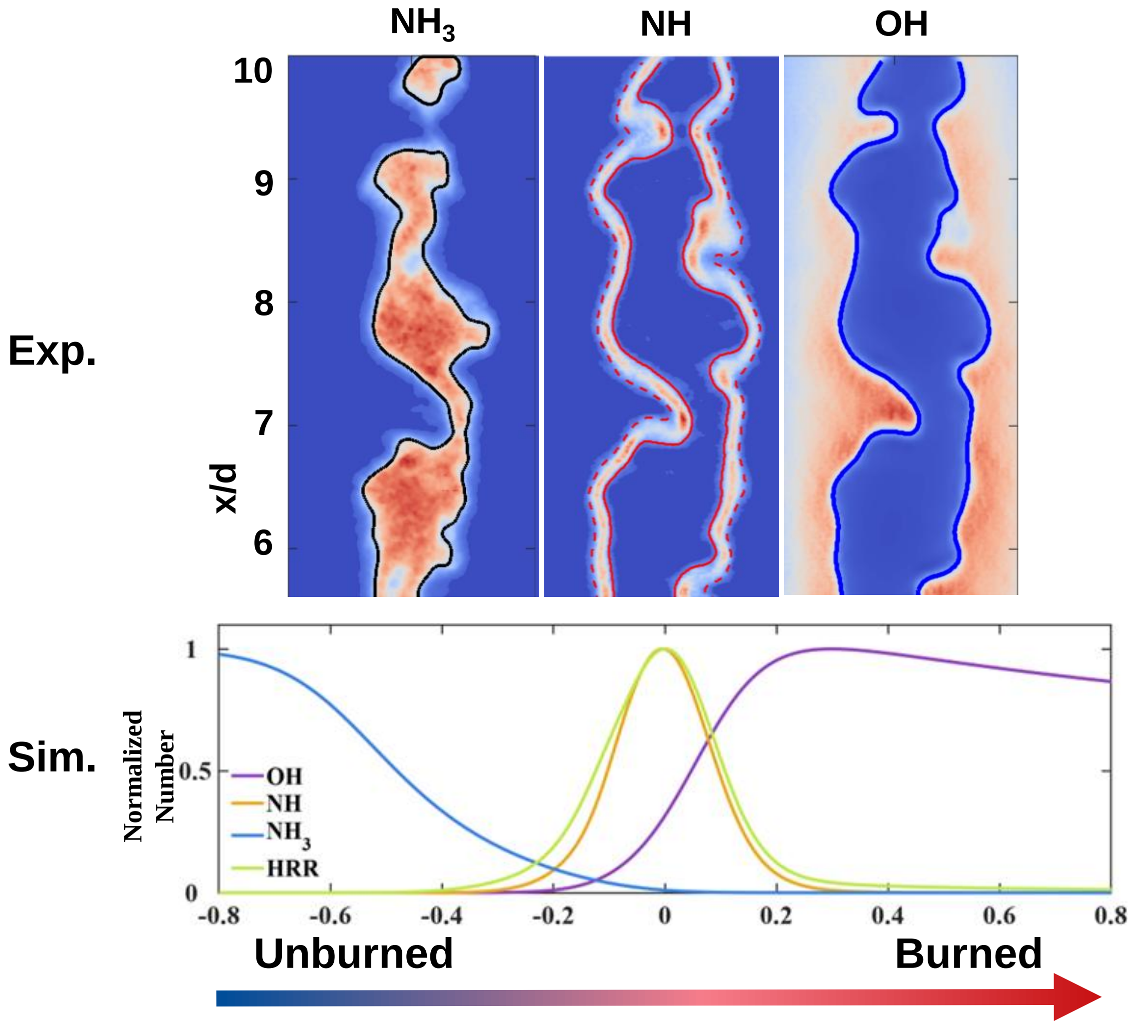
- ***How are they disturbed by turbulence?***

Q2: How can we visualize the **reaction zone containing multiple species**, and how are they modified by differential diffusion and turbulence?

Detailed Flame Structures

What do we know and what can we measure?

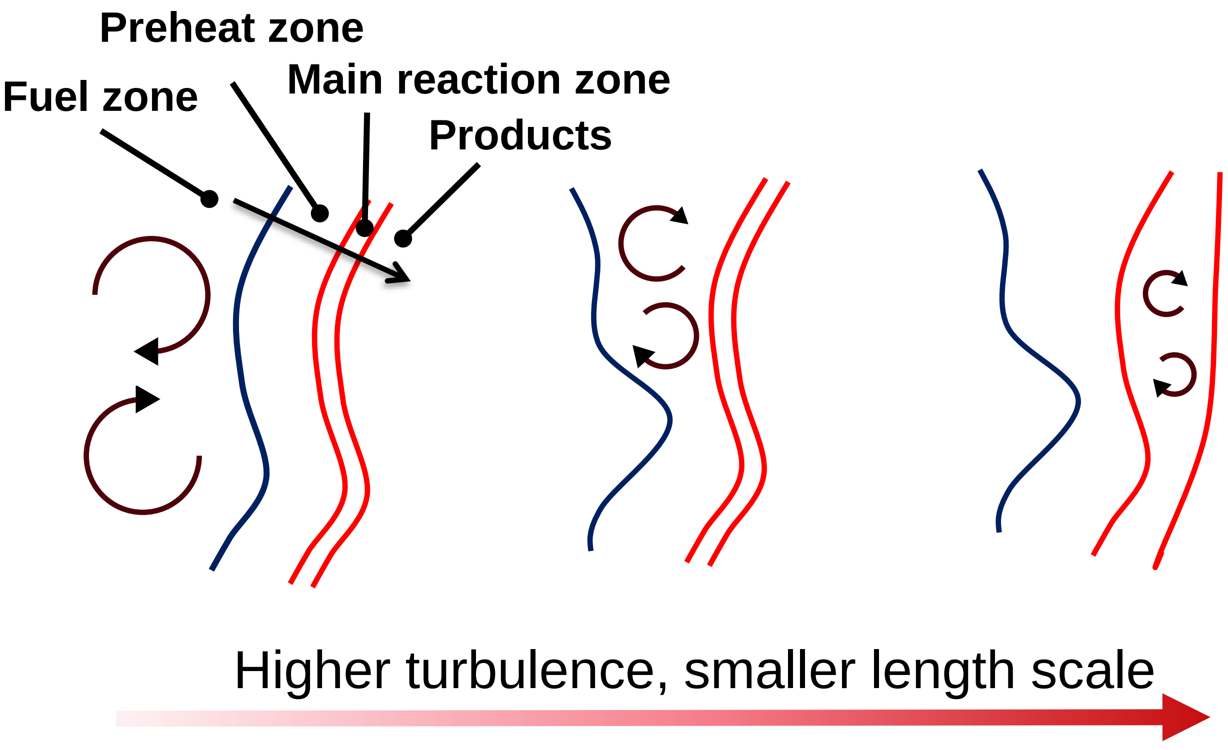


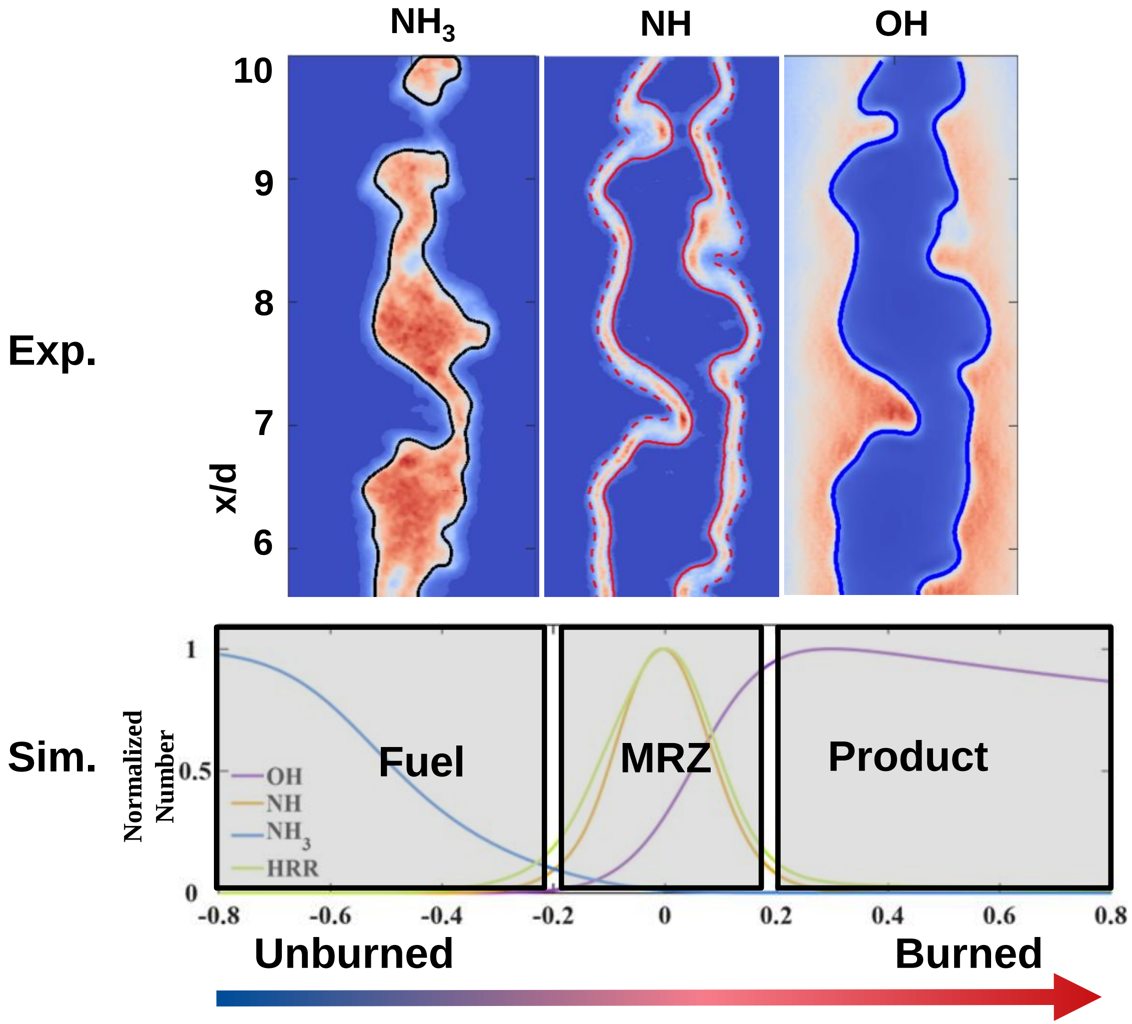


[24] **Z. Wang**, *PhD thesis.* 2025 SUSTech

Detailed Flame Structures

What do we know and what can we measure?

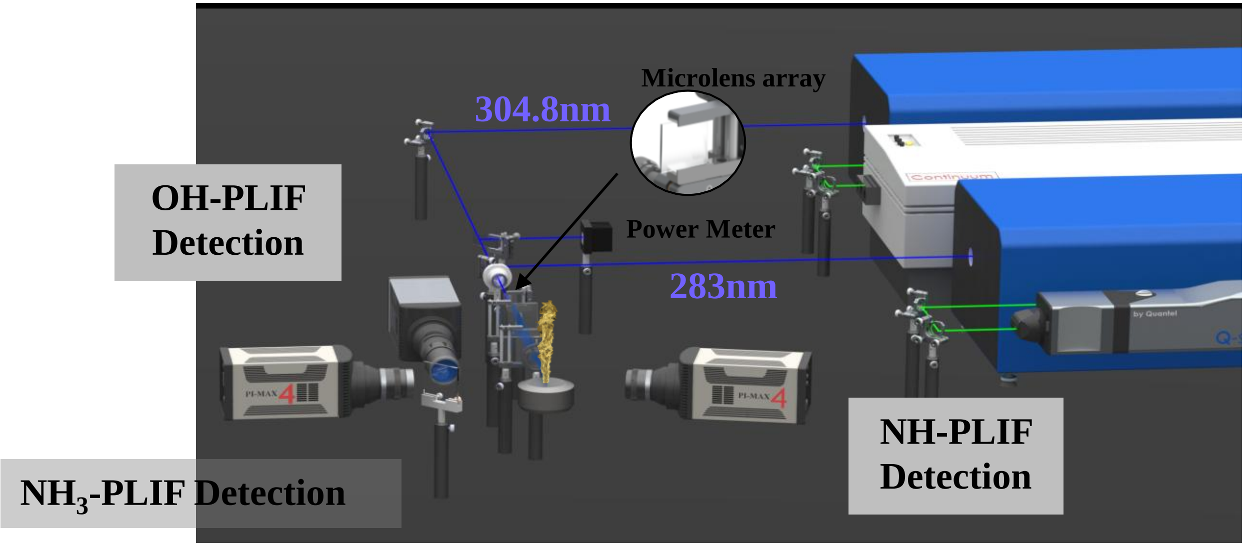




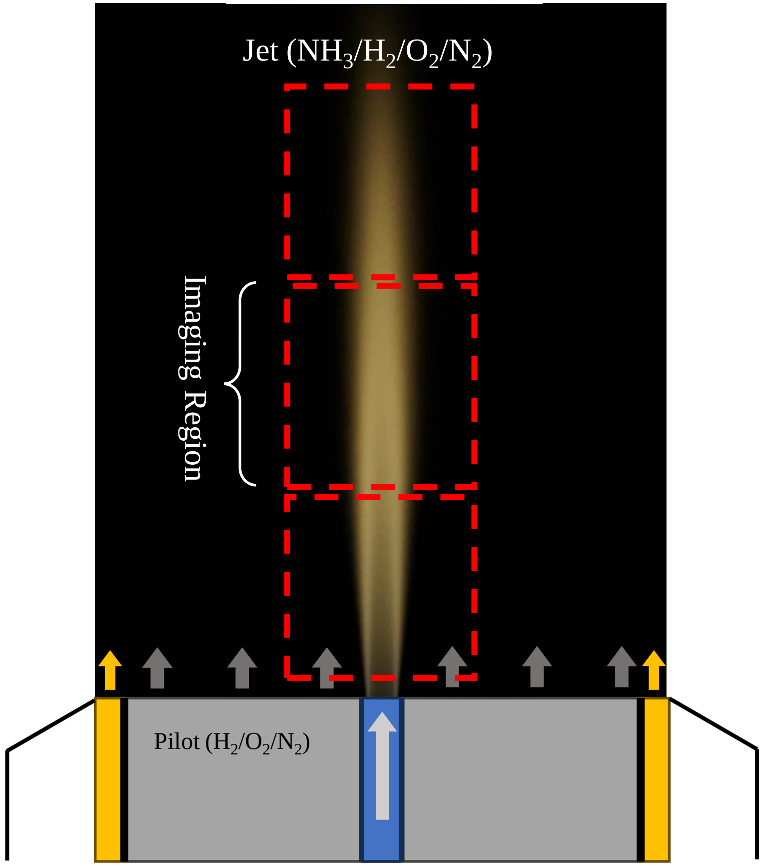
[24] **Z. Wang**, *PhD thesis.* 2025 SUSTech

Multi-scalar LIF Imaging

Simultaneous NH_3, NH and OH



Prof. Bo Zhou, SUSTech 2023



Flame cases

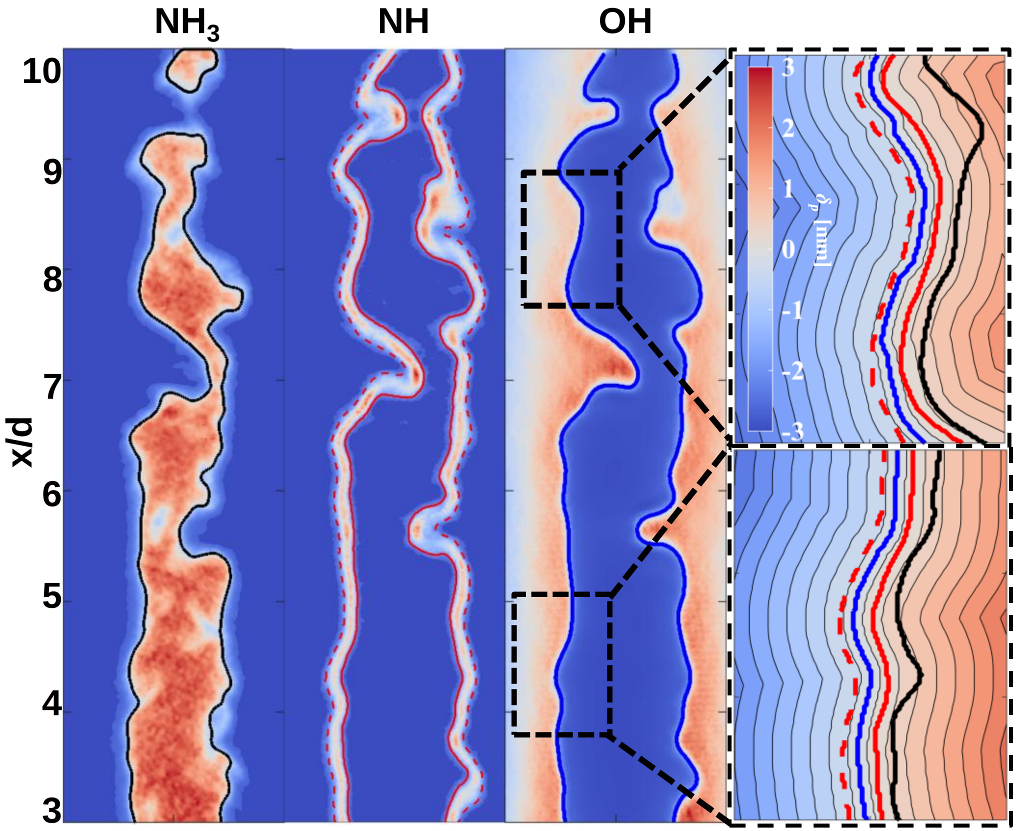
Cases	ϕ	H_2/ NH_3	S_L(cm/s)	U_0 (m/s)	*Le*	l_F(mm)	*Ka*
OL-H20	0.72	20/80	30.8	20-80	0.98	0.53	5-39
OL-H45	0.48	45/55		20-120	0.86	0.46	5-67
OL-H70	0.36	70/30		20-180	0.69	0.47	5-125

[25] **Z. Wang** et al., *Proc. Combust. Inst.* 40(1-4) (2024) 105436

Detailed Flame Structures

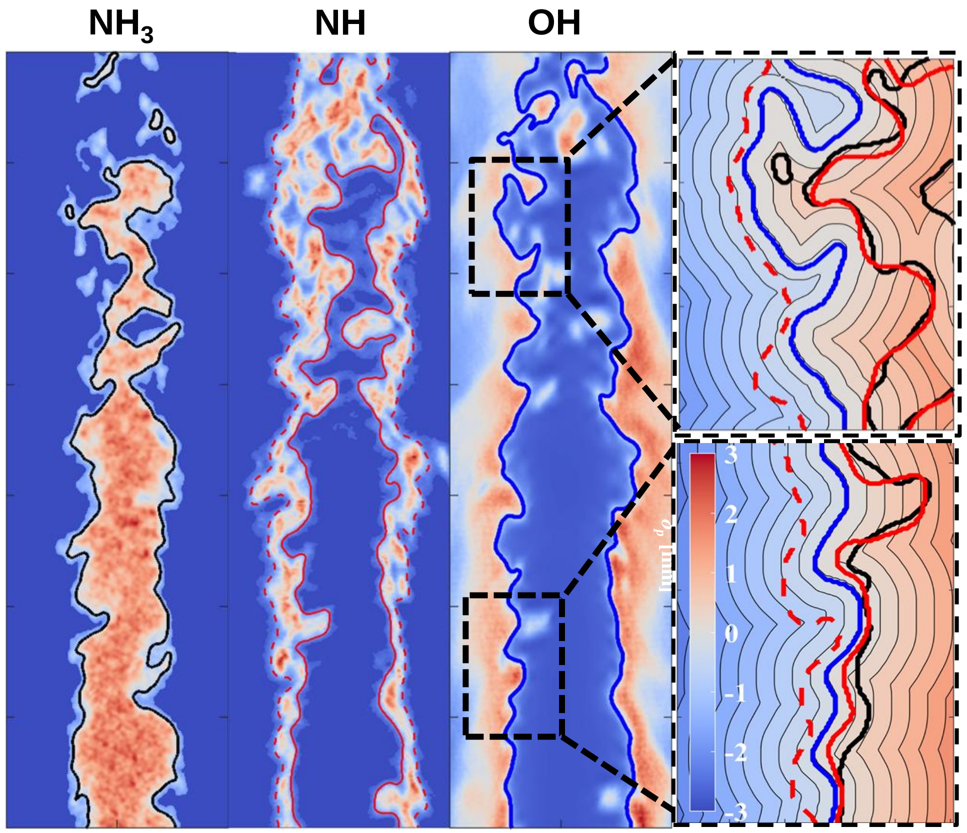
What is turbulence doing?

OL-H20, U_0=20m/s



Parallel iso-contours

OL-H70, U_0=180m/s

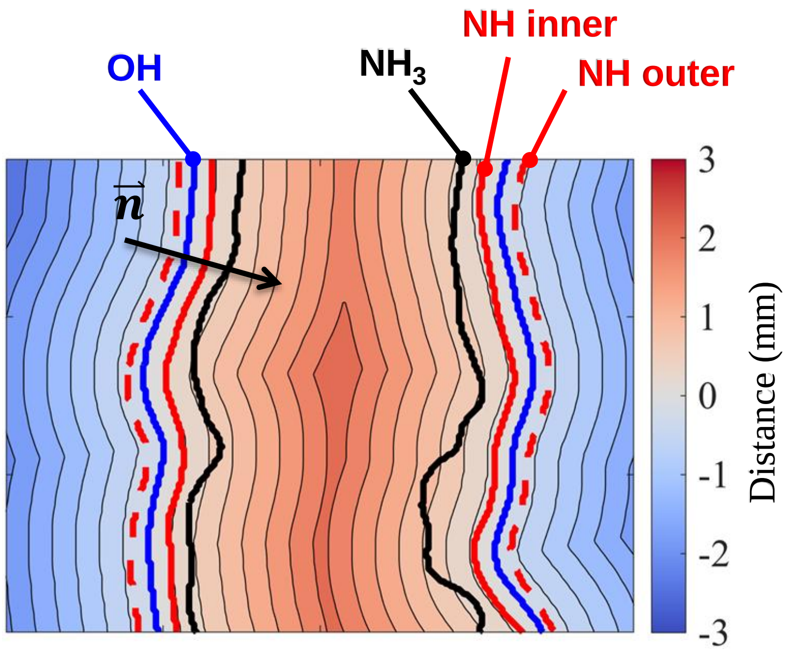


Mismatched iso-contours

[25] **Z. Wang** et al., *Proc. Combust. Inst.* 40(1-4) (2024) 105436

Scalar Parallelism

Take-aways



$$P(\delta_p) = \frac{\sum_{f=1}^{N} p_f(\delta_p)}{\sum_{f=1}^{N} \int_{-\infty}^{+\infty} p_f(\delta_p)\, d\delta_p}$$

Detailed analysis in Ref. [25]

Take-away messages:

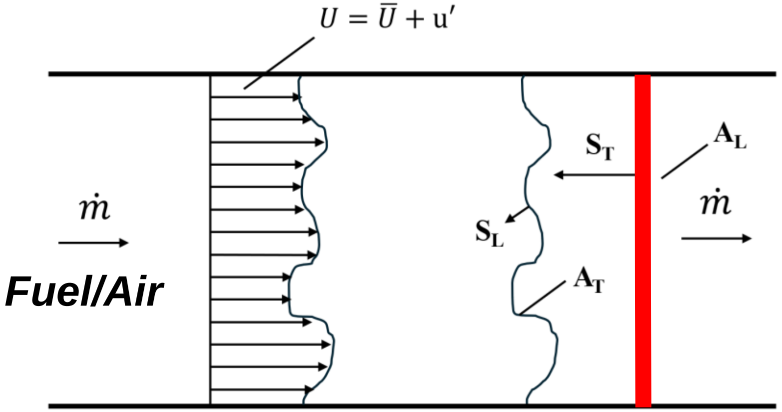
- NH layer is broadened at high turbulence
- An increase in u' or *Ka* **destroys** parallelism between the selected iso-contours (i.e., NH$_3$, inner NH, and outer NH) and the OH baseline
- A decrease in *Le* number **mitigates** this trend

What about global turbulent flame speed calculation?

[25] **Z. Wang** et al., *Proc. Combust. Inst.* 40(1-4) (2024) 105436

Turbulent Flame Speed

One definition



- Based on mass conservation:

$$S_{T,G,\alpha} = \frac{\dot{m}_R}{\rho_R A_\alpha}$$

- To investigate the dependency on the time-averaged iso-surface (A_α) of a selected scalar α (NH_3, NH, OH).

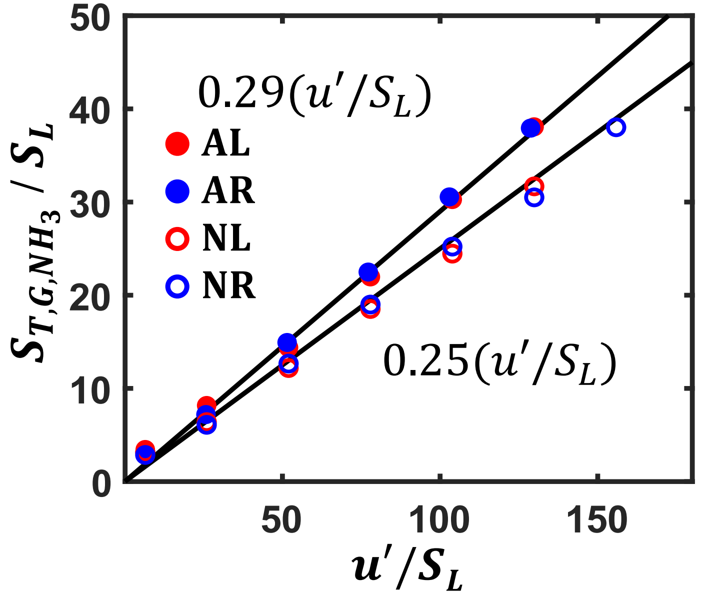
Flame cases

	Cases	ϕ	NH_3/H_2	U_0 (m/s)	*Le*	S_L (cm/s)	l_F (mm)	*Ka*
***A*: Normal air**	AL-H45	0.55	55/45	5-100	0.83	7.7	1.4	64-715
	AR-H45	2.41			1.43		2.18	80-892
***N*: N_2 diluted air**	NL-H45	0.57	55/45	5-100	0.83	7.7	1.39	64-712
	NR-H45	2.14		5-120	1.39		2.07	78-1143

[26] **X. Li, Z. Wang** et al., *Proc. Combust. Inst.* 40(1-4) (2024) 105541

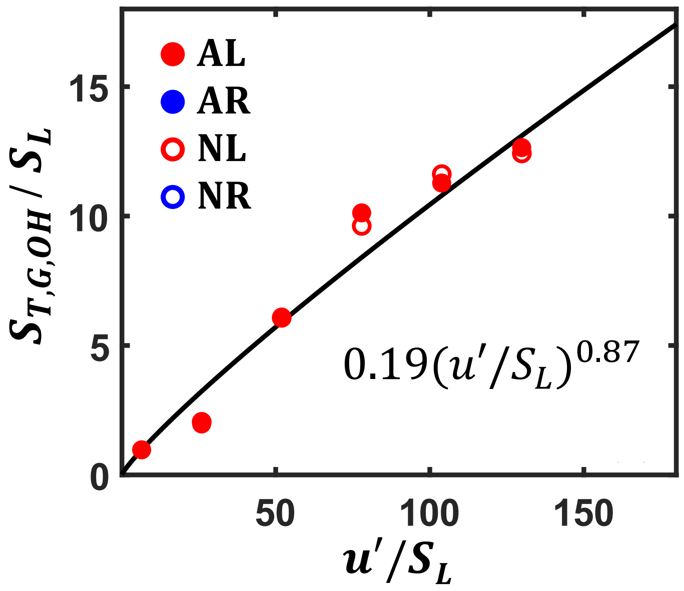
Turbulent Flame Speed

Scaling $S_{T,G,\alpha}/S_L = a(u'/S_L)^b$



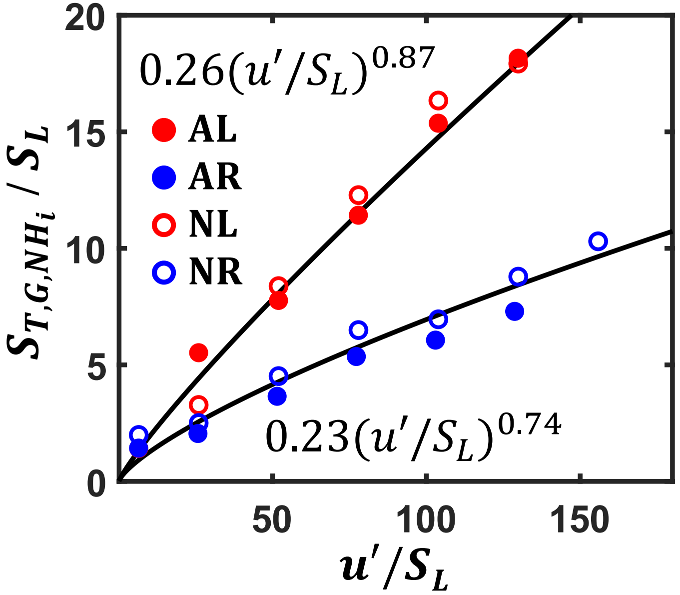
NH_3-based S_T

- Nearly linear to u'/S_L
- Insensitive to *Le* number



OH-based S_T

- Quantitatively different scaling



NH-based S_T

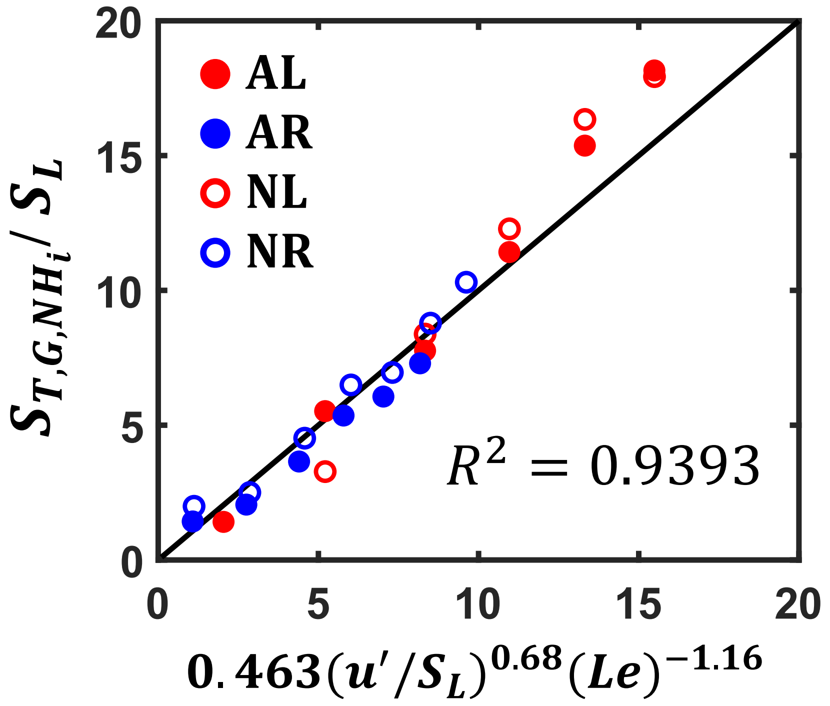
- Significant effects of *Le* number (differential diffusion)

[26] **X. Li, Z. Wang** et al., *Proc. Combust. Inst.* 40(1-4) (2024) 105541

Turbulent Flame Speed

A better scaling?

$$S_{T,G,\alpha}/S_L = a\ (u'/S_L)^b\ (Le)^c$$



Take-away messages:

- Turbulent flame speed S_T calculation depends on the choice of isoscalars (reaction zone structure)
- Empirical scaling of S_T should consider turbulent intensity u' and *Le* number
- Differential diffusion effects remain at high turbulence→ Lean burns faster

Why do the lean and rich flames burn differently?

[26] **X. Li, Z. Wang** et al., *Proc. Combust. Inst.* 40(1-4) (2024) 105541

Q3: How to quantify the **thermochemical states** of stratified flames, and what can we learn from the data?

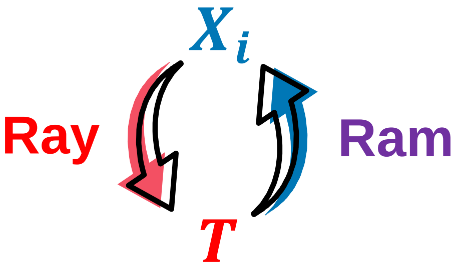
Spontaneous 1D Raman/Rayleigh Scattering

- Temperature (Ray)
- Number density of major species (Ram)

Temperature (Ray):

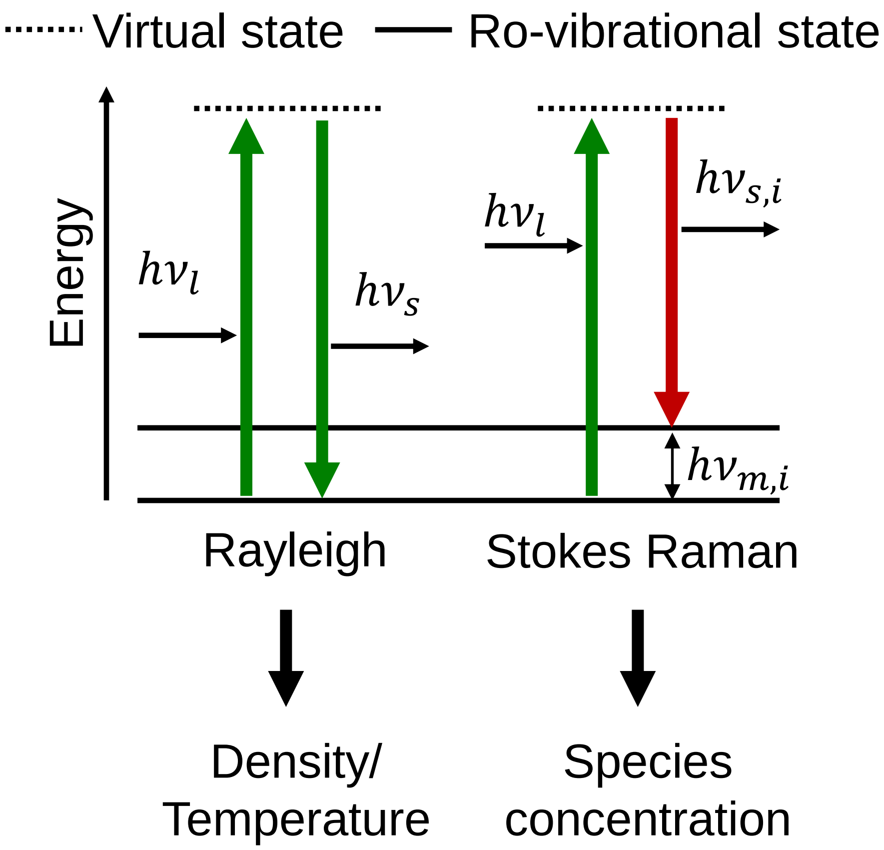
$$S_{Ray} \propto \sum_{i=1}^{n} \boldsymbol{X_i}\, \sigma_{Ray,i} \cdot I_l \cdot N$$

$$N \propto \frac{1}{\boldsymbol{T}}$$



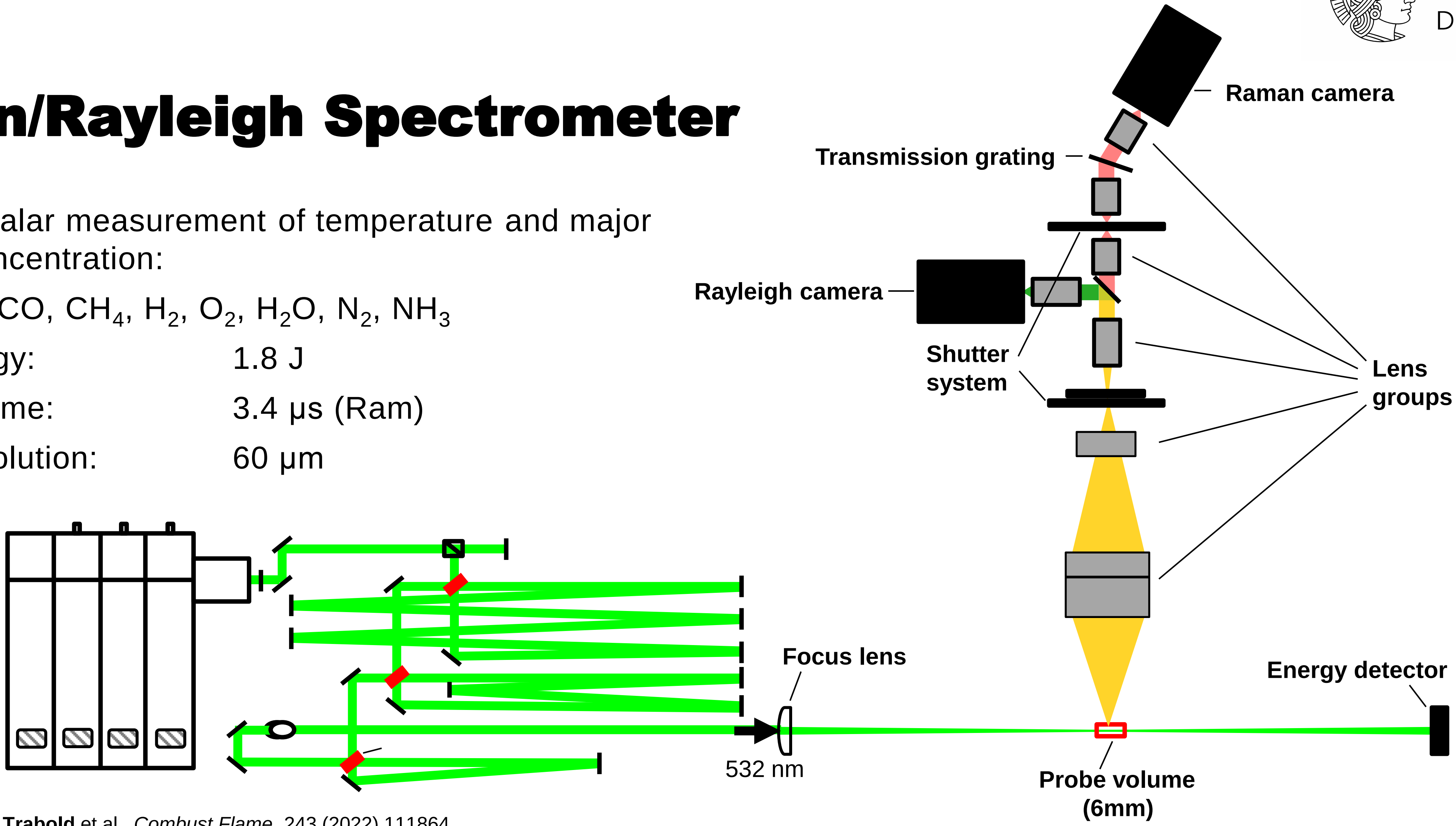
Number density of species *i* (Ram):

$$S_{Ram,i} \propto \sigma_{Ram,i}(\boldsymbol{T}) \cdot I_l \cdot \boldsymbol{X_i} \cdot N$$



Raman/Rayleigh Spectrometer

- 1D multi-scalar measurement of temperature and major species concentration:
    - CO_2, CO, CH_4, H_2, O_2, H_2O, N_2, NH_3
- Pulse energy: 1.8 J
- Exposure time: 3.4 µs (Ram)
- Spatial resolution: 60 µm



[27] **J. Trabold** et al., *Combust Flame*, 243 (2022) 111864
[28] **F. Fuest** et al., *Proc. Combust. Inst.*, 33 (2011) 815–822

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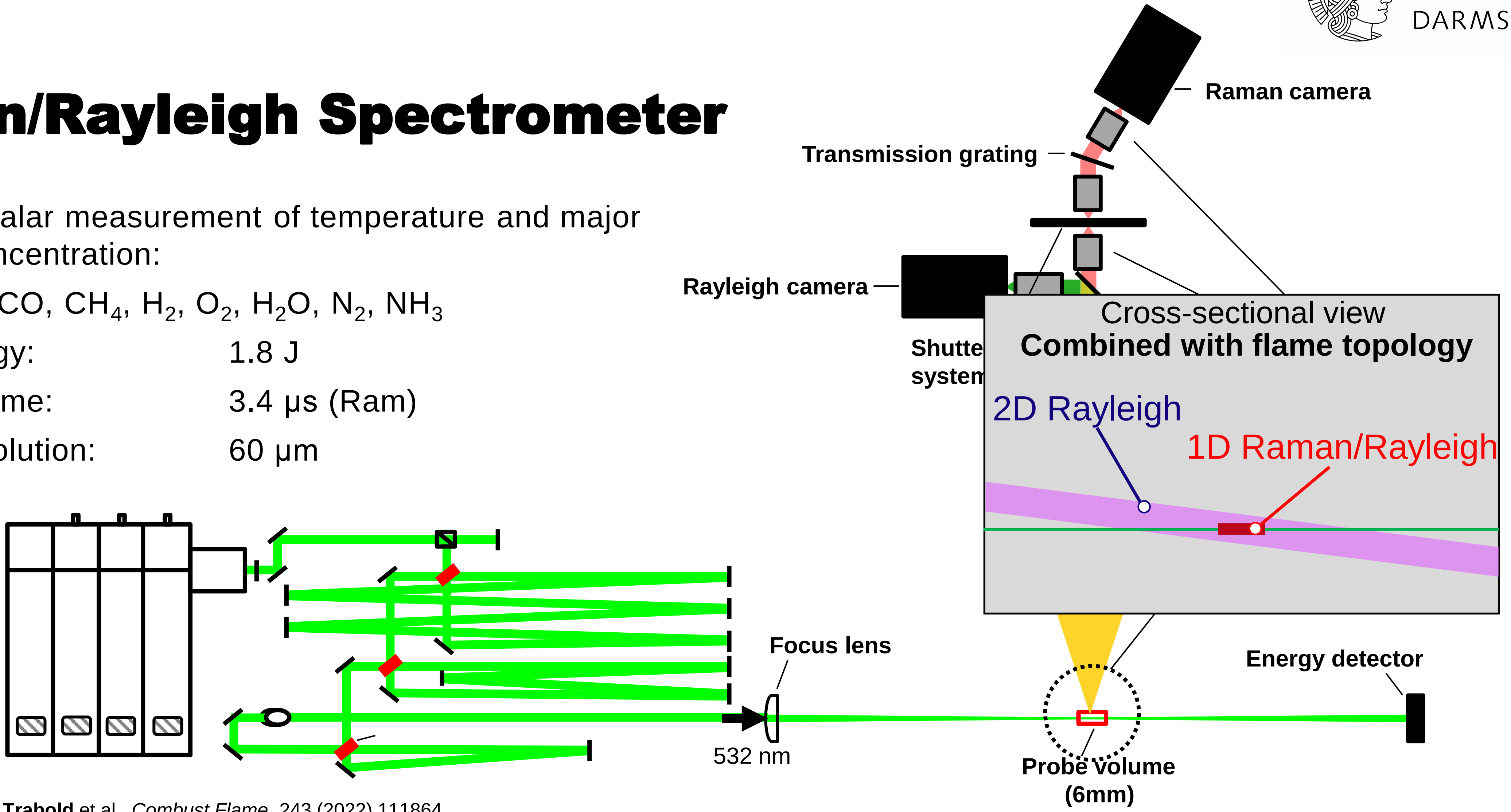

[27] **J. Trabold** et al., *Combust Flame*, 243 (2022) 111864
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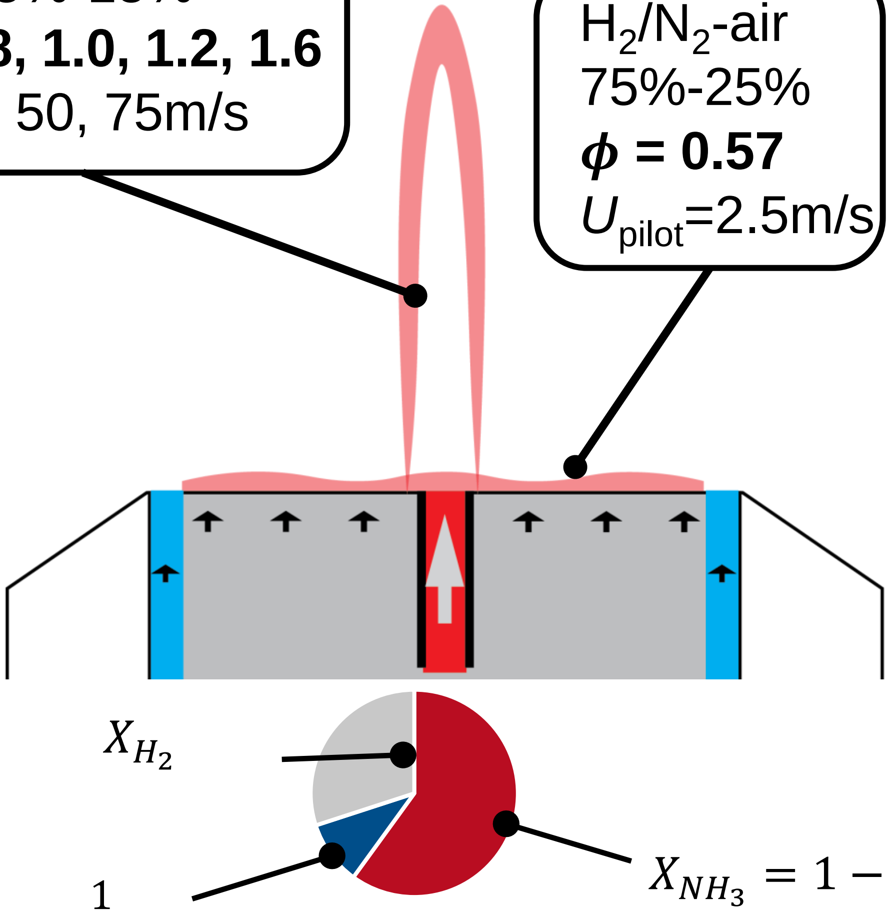
Flame Conditions



$NH_3/H_2/N_2$-air
40%-45%-15%
ϕ = 0.8, 1.0, 1.2, 1.6
U_0=25, 50, 75m/s

H_2/N_2-air
75%-25%
ϕ = 0.57
U_{pilot}=2.5m/s

X_{H_2}

$X_{NH_3} = 1 - \frac{4}{3} X_{H_2}$

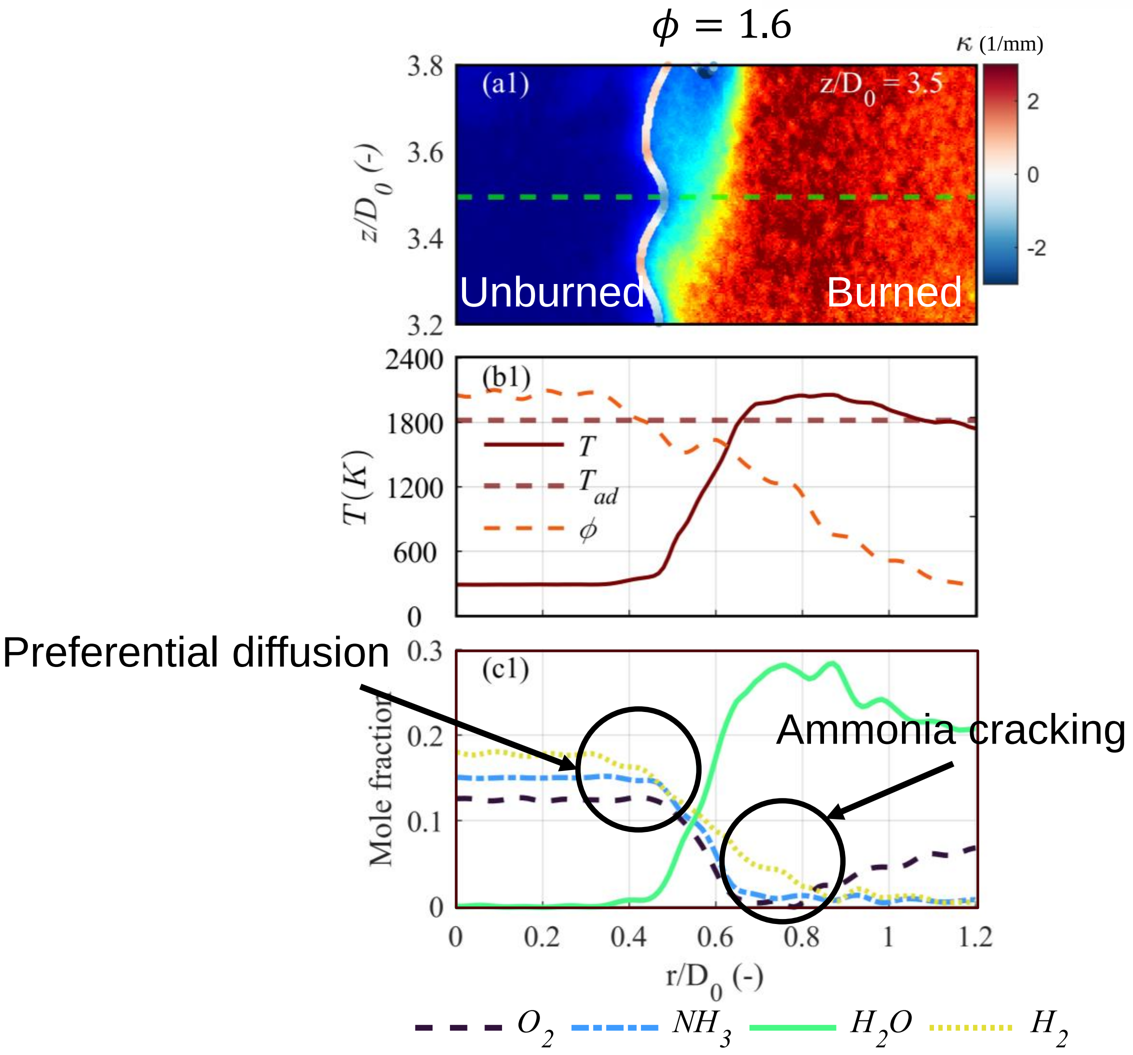
$X_{N_2} = \frac{1}{3} X_{H_2}$

Probe volume
z/D=3.5

Internal Flame Structures

Unburned → **Burned**

- **Low-temperature:** early decreasing of H_2 compared to NH_3 **in rich flames**
- **High-temperature:** H_2 remains, NH_3 is completely consumed



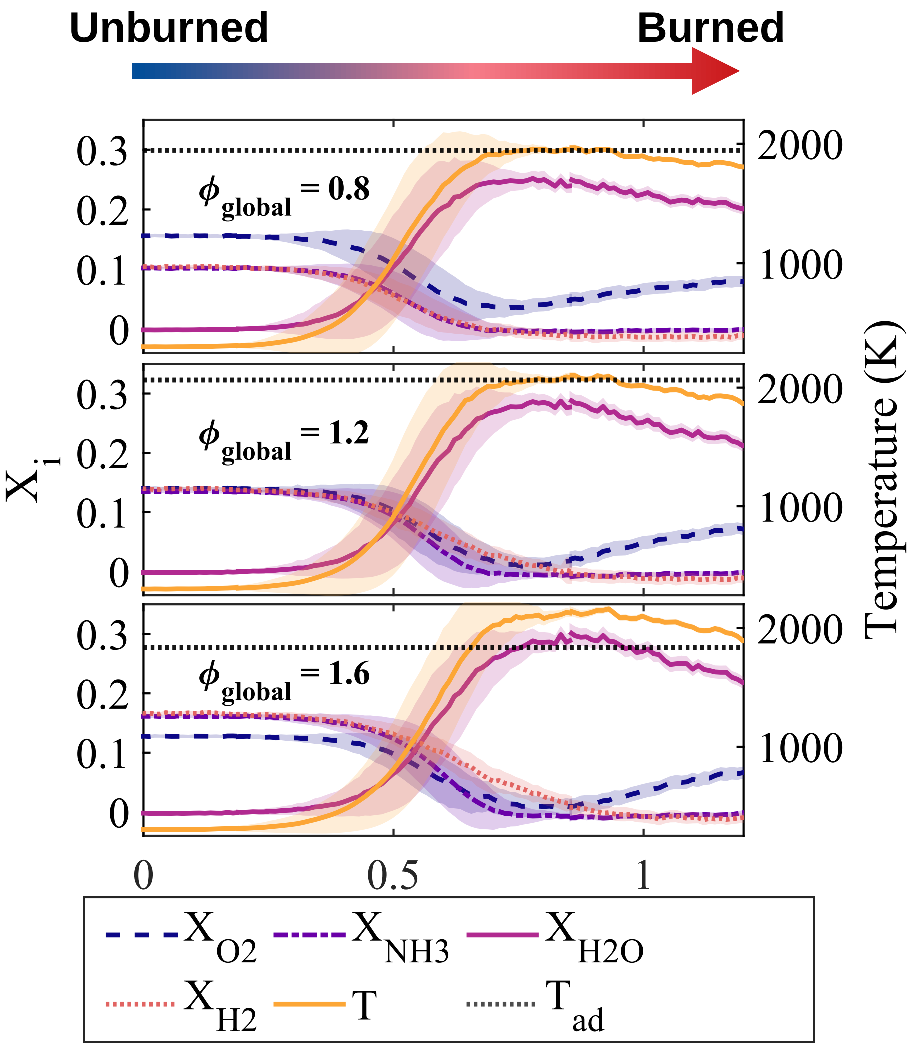
Preferential diffusion

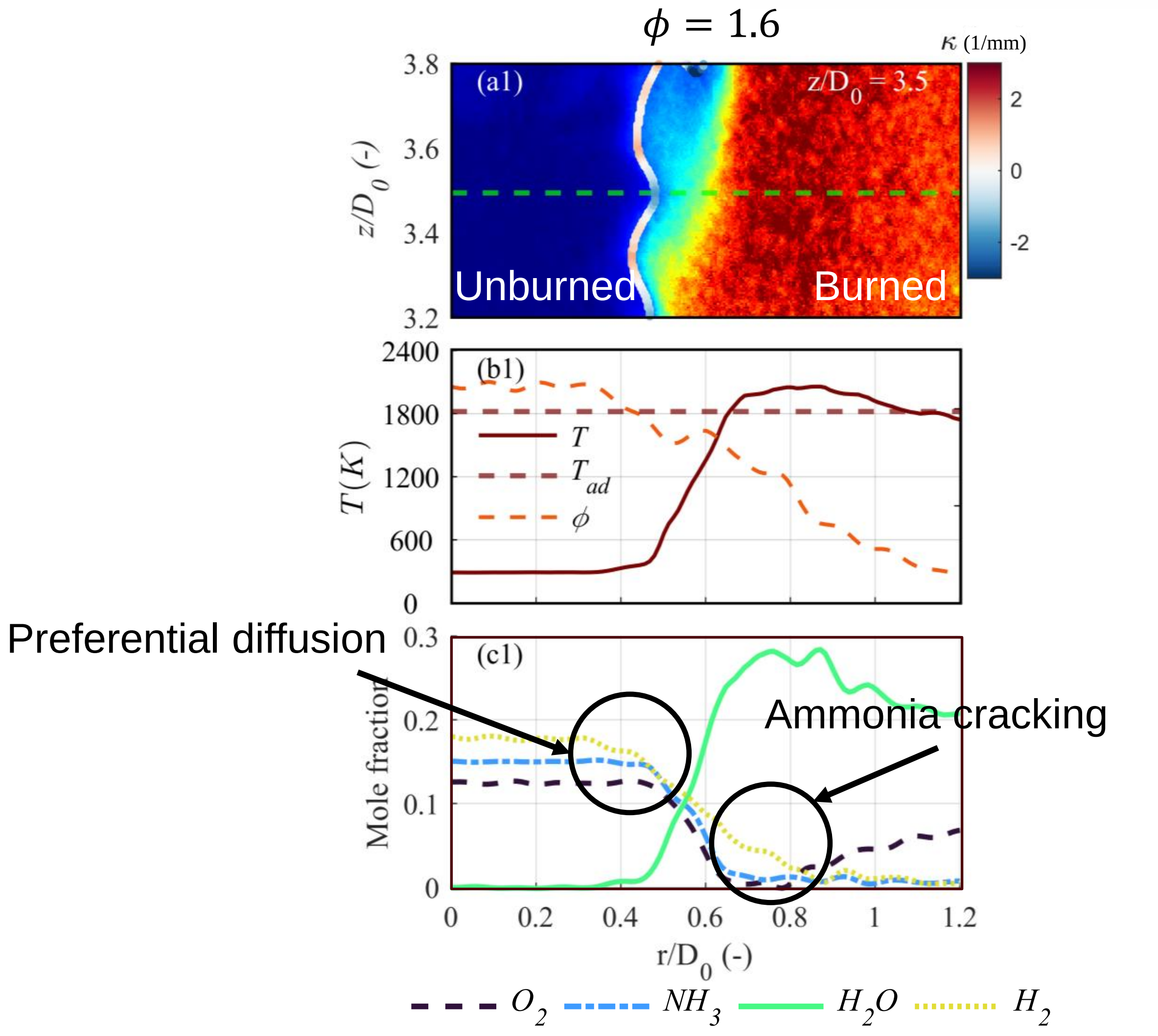
Ammonia cracking

[29] **R. Schultheis** et al., *Proc. Combust. Inst.* 40(1-4) (2024) 105571

Internal Flame Structures

- **Low-te** compar
- **High-te** consum





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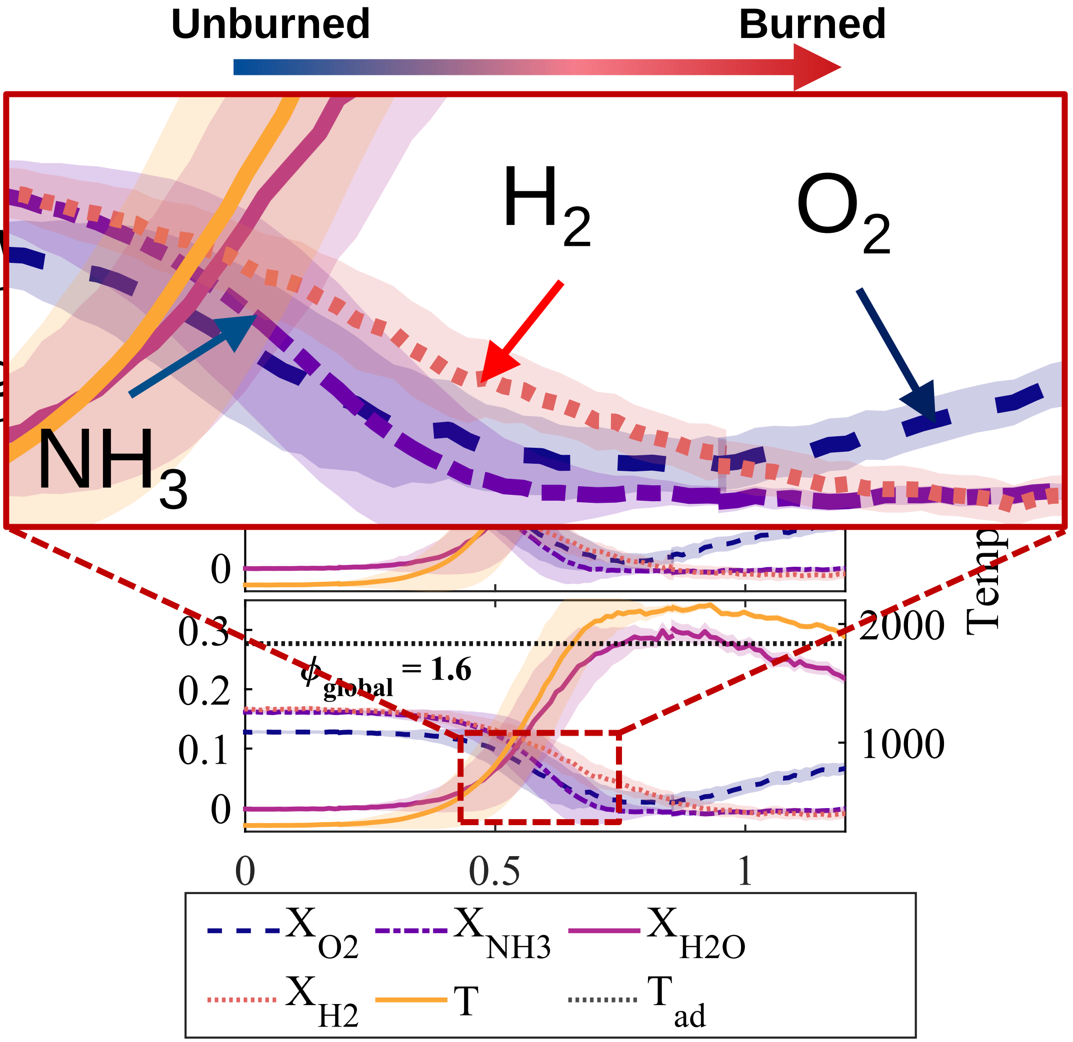
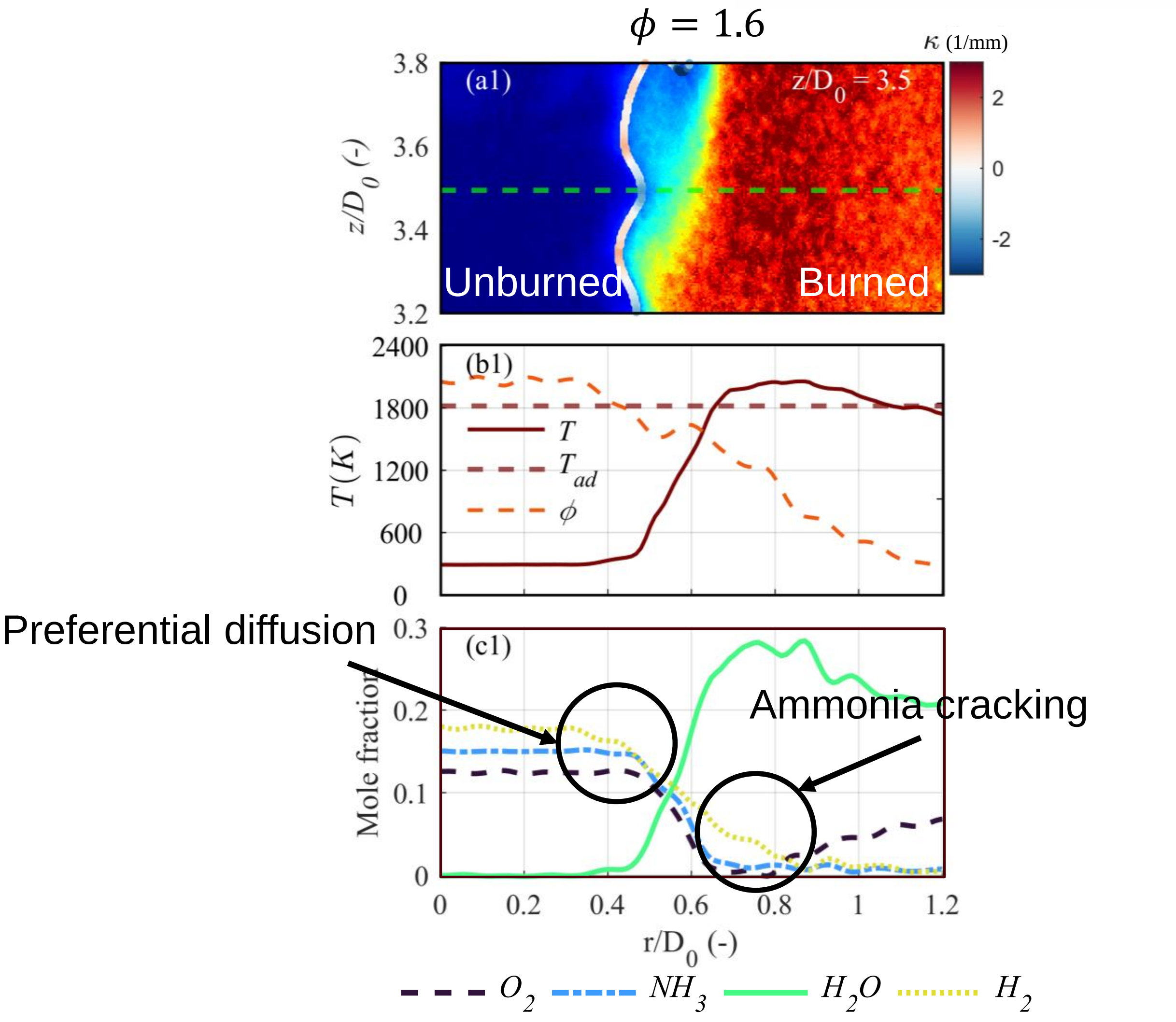
Internal Flame Structures

- **Lo** cor
- **Hig** cor





[29] **R. Schultheis** et al., *Proc. Combust. Inst.* 40(1-4) (2024) 105571

Preferential Diffusion

Mole fractions in temperature space

- H_2 faster diffusion at low temperature
  - Depends on curvature
- NH_3 consumption is linear to temperature
  - Insensitive to ϕ and κ
- Significant amount of H_2 at high temperature
  - NH_3 fully decomposed, no NH_3 slip!

Unpublished Results

[30] **R. Schultheis** et al., *Combust. Flame* (2026) Under preparation

Preferential Diffusion

NH_3:H_2 molar ratio

- Preferential diffusion at low temperature
- Turbulence mitigates it
- NH_3 consumption is faster at high temperature
- The “*turnover*" point shifts to lower temperature

Unpublished Results

[30] **R. Schultheis** et al., *Combust. Flame* (2026) Under preparation

NH_3-H_2 interactions

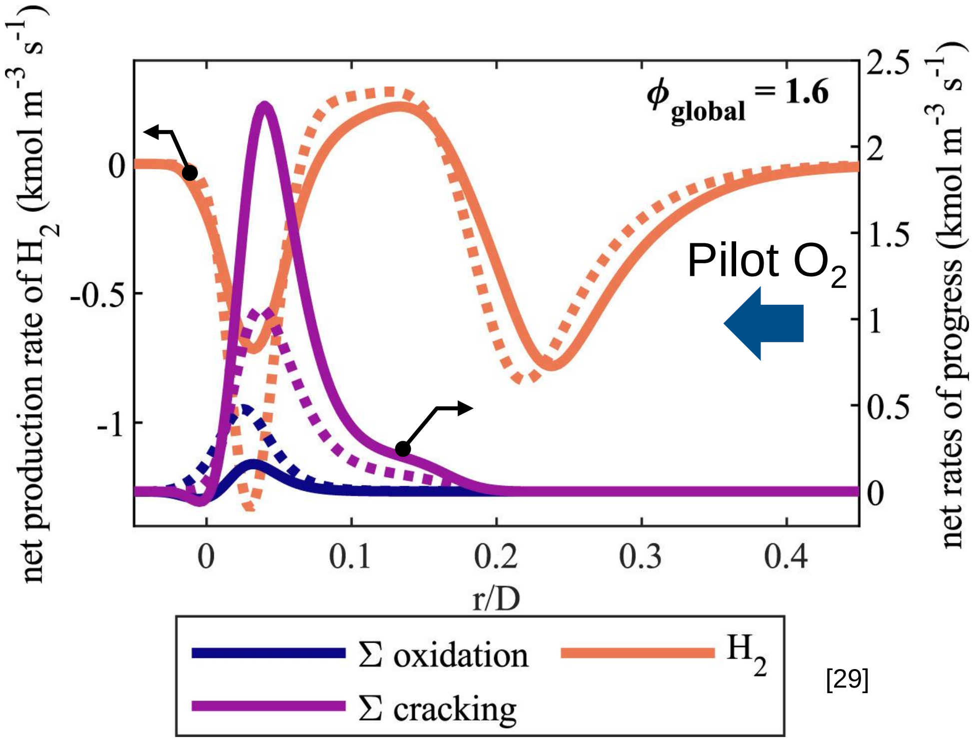
Undelaying pathways

- 1D counter-flow simulations
- Different reaction mechanisms[9,30]
- Rate of NH_3 cracking:

$$\mathrm{NH_3} \rightleftharpoons \mathrm{H} + \mathrm{NH_2}$$
$$\mathrm{H} + \mathrm{NH_3} \rightleftharpoons \mathrm{H_2} + \mathrm{NH_2}$$
$$\mathrm{H} + \mathrm{NH_2} \rightleftharpoons \mathrm{H_2} + \mathrm{NH}$$

- Rate of NH_3 oxidation

$$\mathrm{NH_3} + \mathrm{O_2} \rightleftharpoons \mathrm{HO_2} + \mathrm{NH_2}$$
$$\mathrm{NH_3} + \mathrm{O} \rightleftharpoons \mathrm{NH_2} + \mathrm{OH}$$

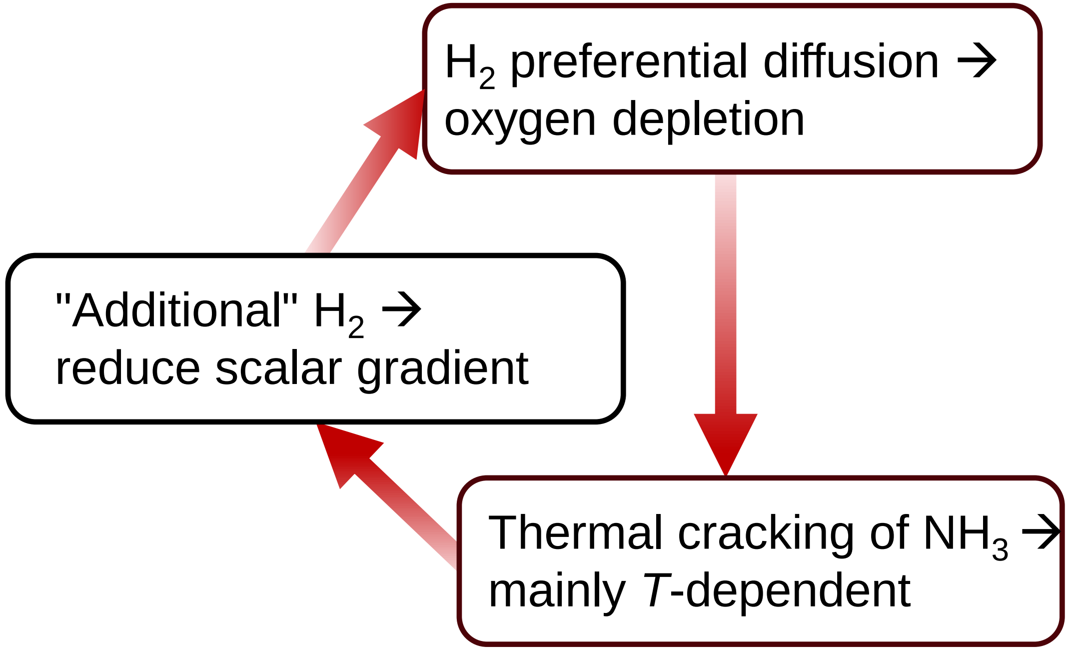


[29]

[9] **A. Stagni**, *Chem. Eng. J.*, 471 (2023), 144577
[30] **X. Han** et al. *Combust. Flame*, 213 (2020), 1-13
[31] **P. Glarborg** et al., *Fuel Communication.* 10 (2022) 100049
[29] **R. Schultheis** et al., *Proc. Combust. Inst.* 40(1-4) (2024) 105571

NH_3-H_2 interactions

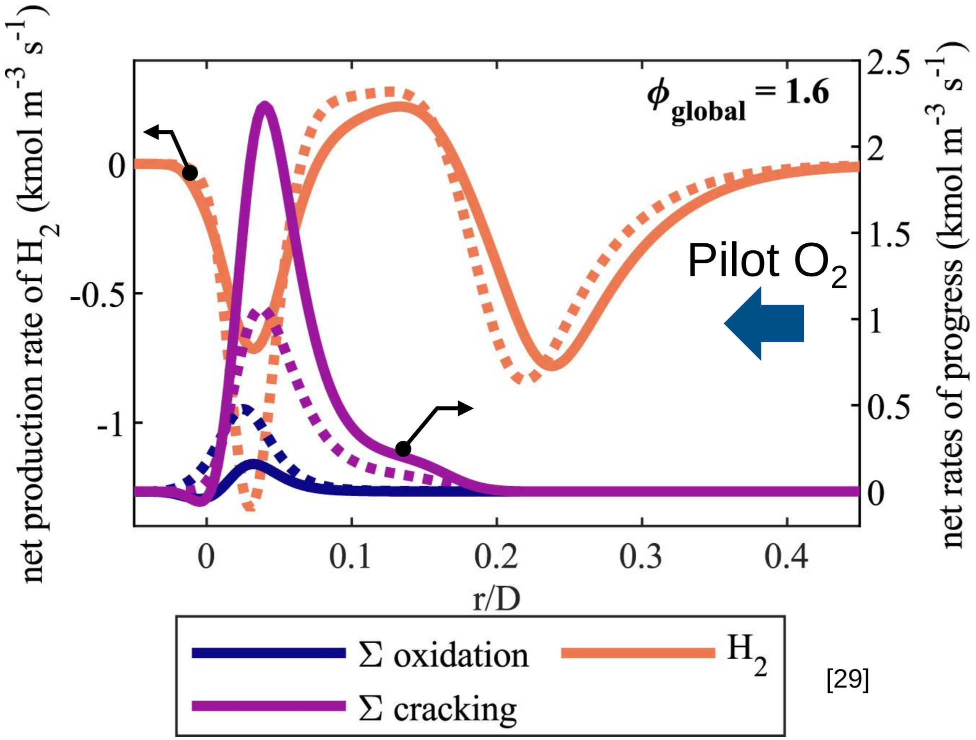
Undelaying pathways



H_2 preferential diffusion → oxygen depletion

Thermal cracking of NH_3 → mainly *T*-dependent

"Additional" H_2 → reduce scalar gradient



[29]

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[29] R. Schultheis et al., *Proc. Combust. Inst.* 40(1-4) (2024) 105571

Summary and Conclusions

1. **Global Structures**
   - Premixed NH_3/H_2 flames show high resistance to turbulence.
   - OH layer thickness is not broadened by turbulence, but OH intensity and its gradients are influenced

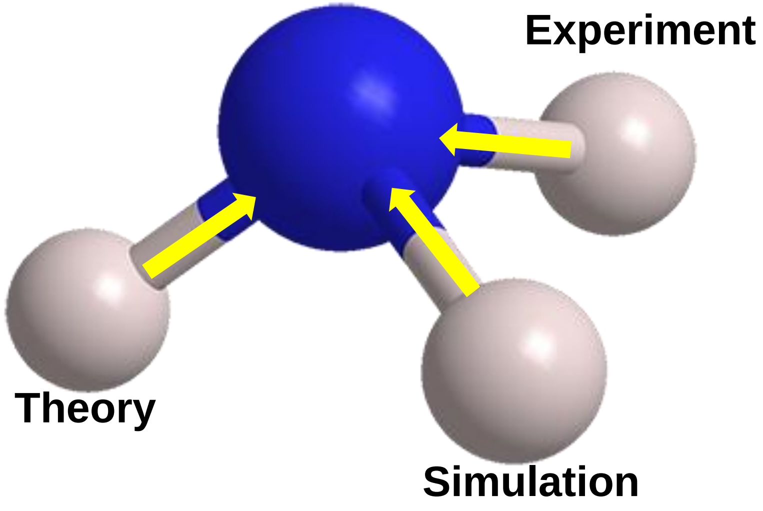
2. **Detailed Structures**
   - Iso-counters (NH_3, NH, OH) are significantly modified by turbulence and *Le* number
   - Turbulence flame speed varies between selected scalars

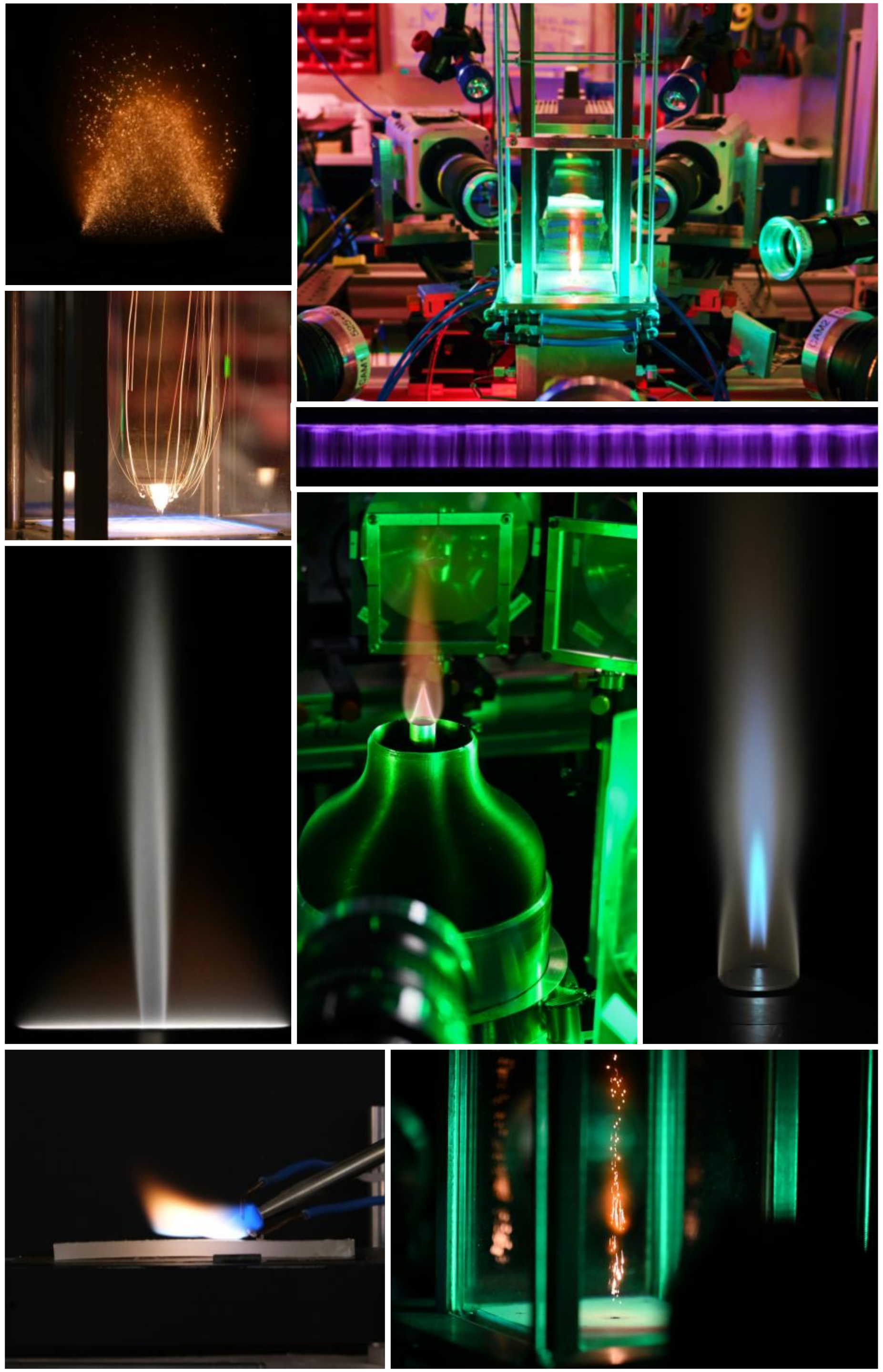
3. **Internal Structures**
   - Preferential diffusion at low temperature
   - Interplay of diffusion, thermal cracking and oxidation

Future research steps

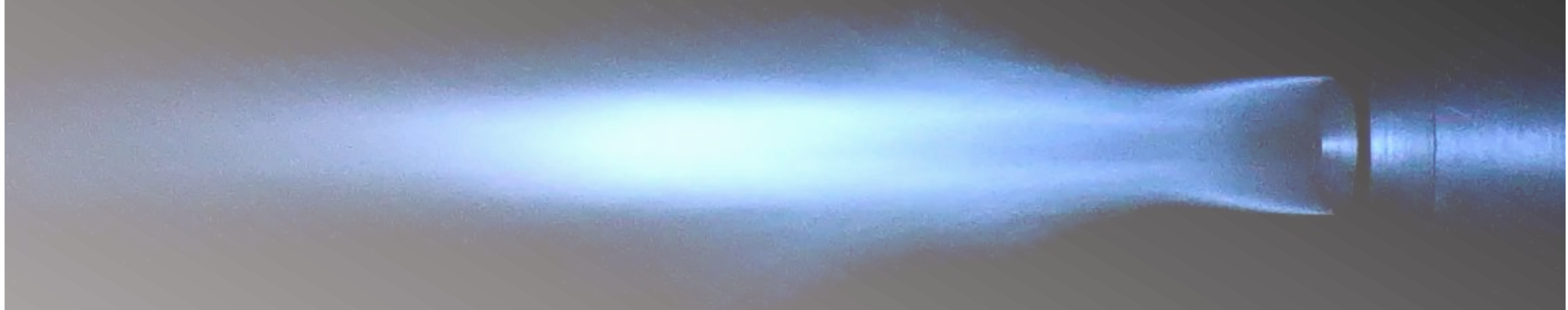
- In-situ NO measurements in turbulent flames
- Flame structures under pressure
- …

Joint Efforts Towards NH_3 Fuel Utilization





Thank You!



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