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DIRECT NUMERICAL SIMULATION OF HYDROGEN AND AMMONIA COMBUSTION

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With contributions from:
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Carbon-Free Fuel Combustion Workshop, March 16 2025

U.S. DEPARTMENT of ENERGY NNSA National Nuclear Security Administration

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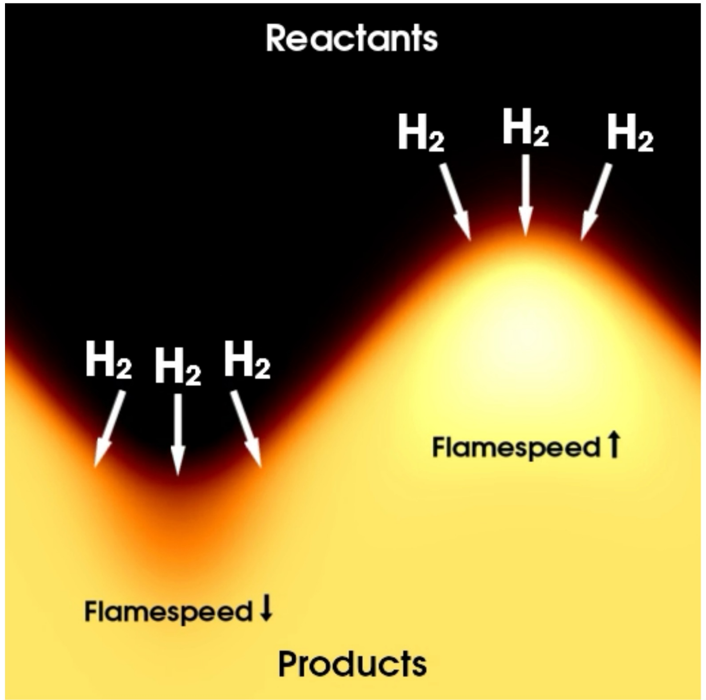
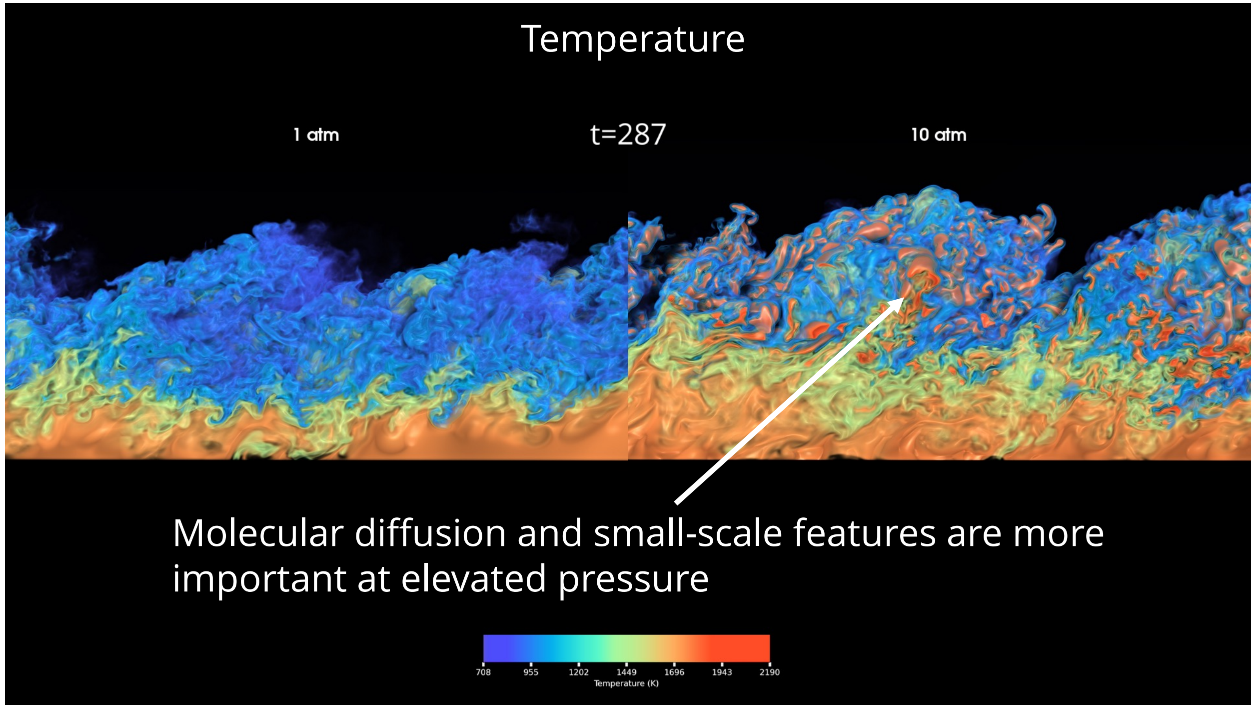
WHY DIRECT NUMERICAL SIMULATION (DNS)?

- DNS fully resolves turbulence-chemistry interaction
- Expensive, <u>but</u> gives full account of physics on the small scale
- Capturing small scales is crucial <u>especially</u> for hydrogen-containing fuels at elevated pressures

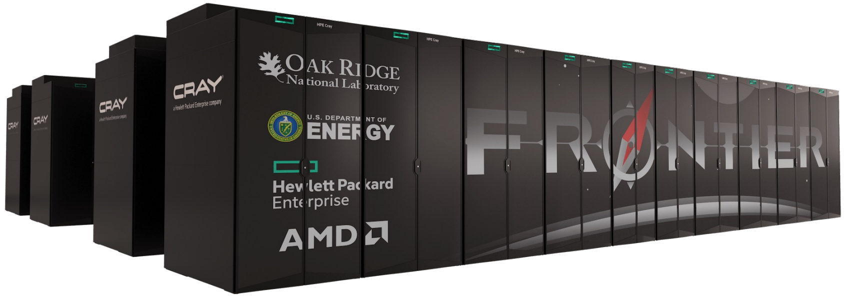
Thermo-diffusive instabilities (for Le<1)



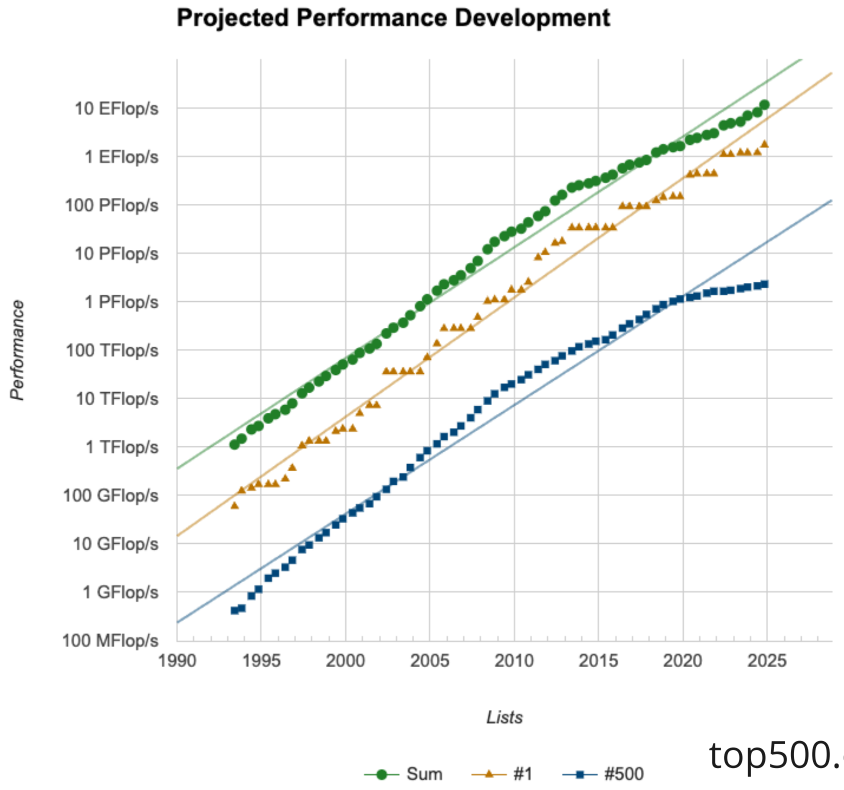
Turbulent flame at 1 and 10 atm



DNS STATE-OF-THE-ART

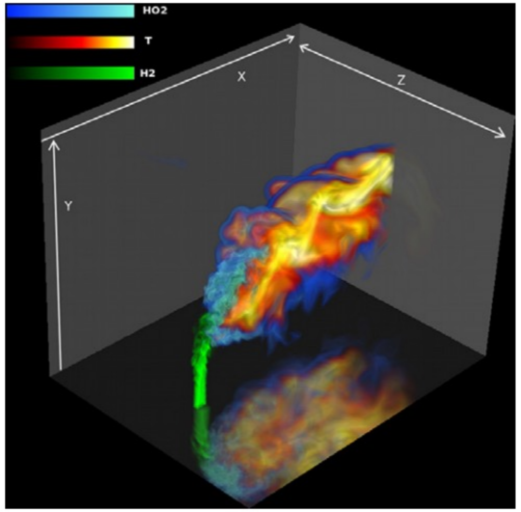


ECP EXASCALE COMPUTING PROJECT



top500.org

- Advancements in computing power and algorithm development have enabled Exascale DNS
- Shift to GPUs posed a challenge in the last 10 years
- Codes used for DNS in this talk:
  - S3D
  - Pele

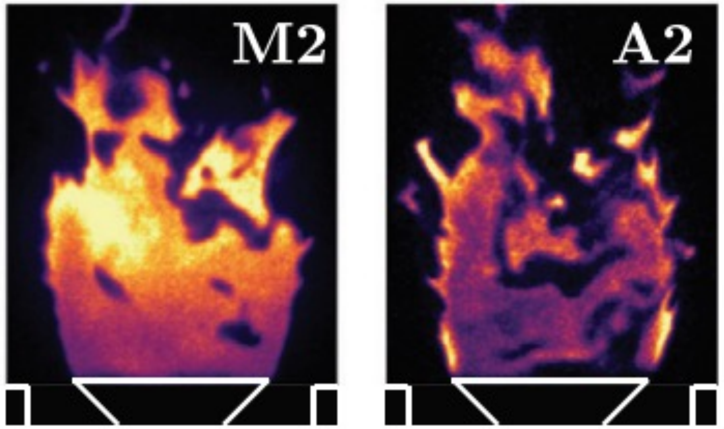


2011: 1.7 billion grid points compressible DNS at atmospheric pressure (Grout et al., PROCI, 2011)
2023: 35 billion grid points low-Mach DNS at high pressure (Rieth et al., PROCI, 2024)

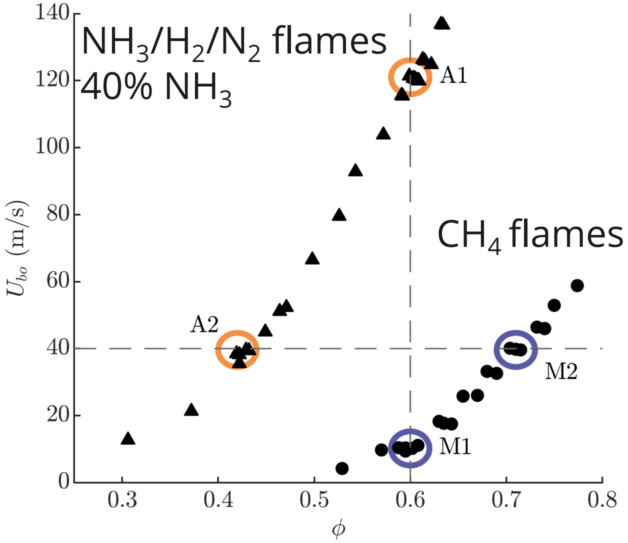
PREMIXED AMMONIA AND HYDROGEN FLAMES

DIFFERENCES BETWEEN $NH_3/H_2/N_2$ AND CH_4 FLAMES - EXPERIMENTS

Experiments

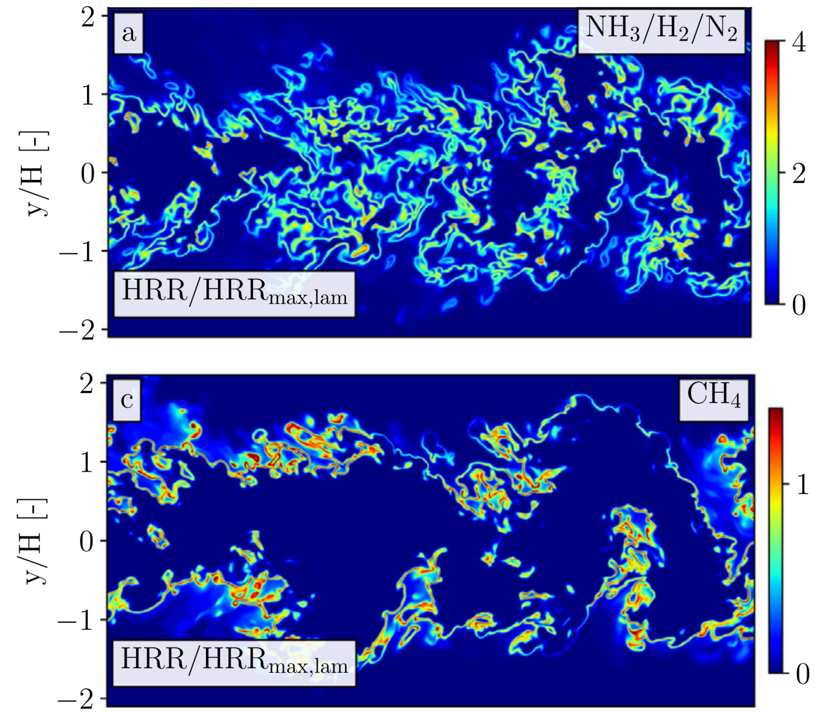


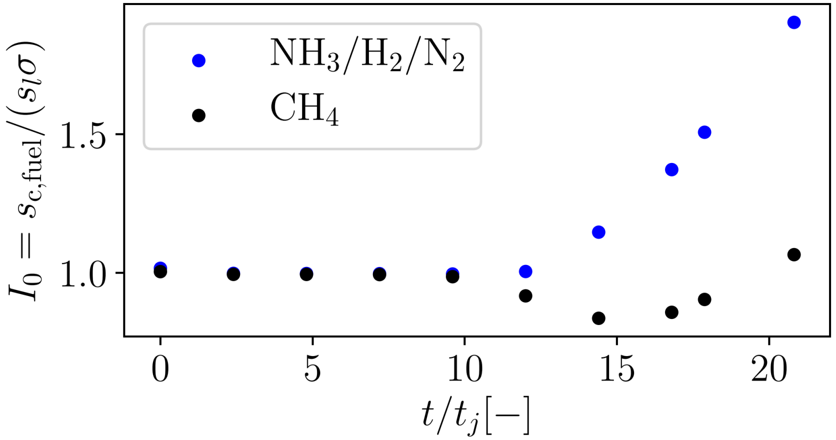
OH PLIF of NH3/H2/N2-air (A2) and methane-air (M2) flames



Wiseman et al., PROCI, 2021.

DNS





Burning rate enhancement

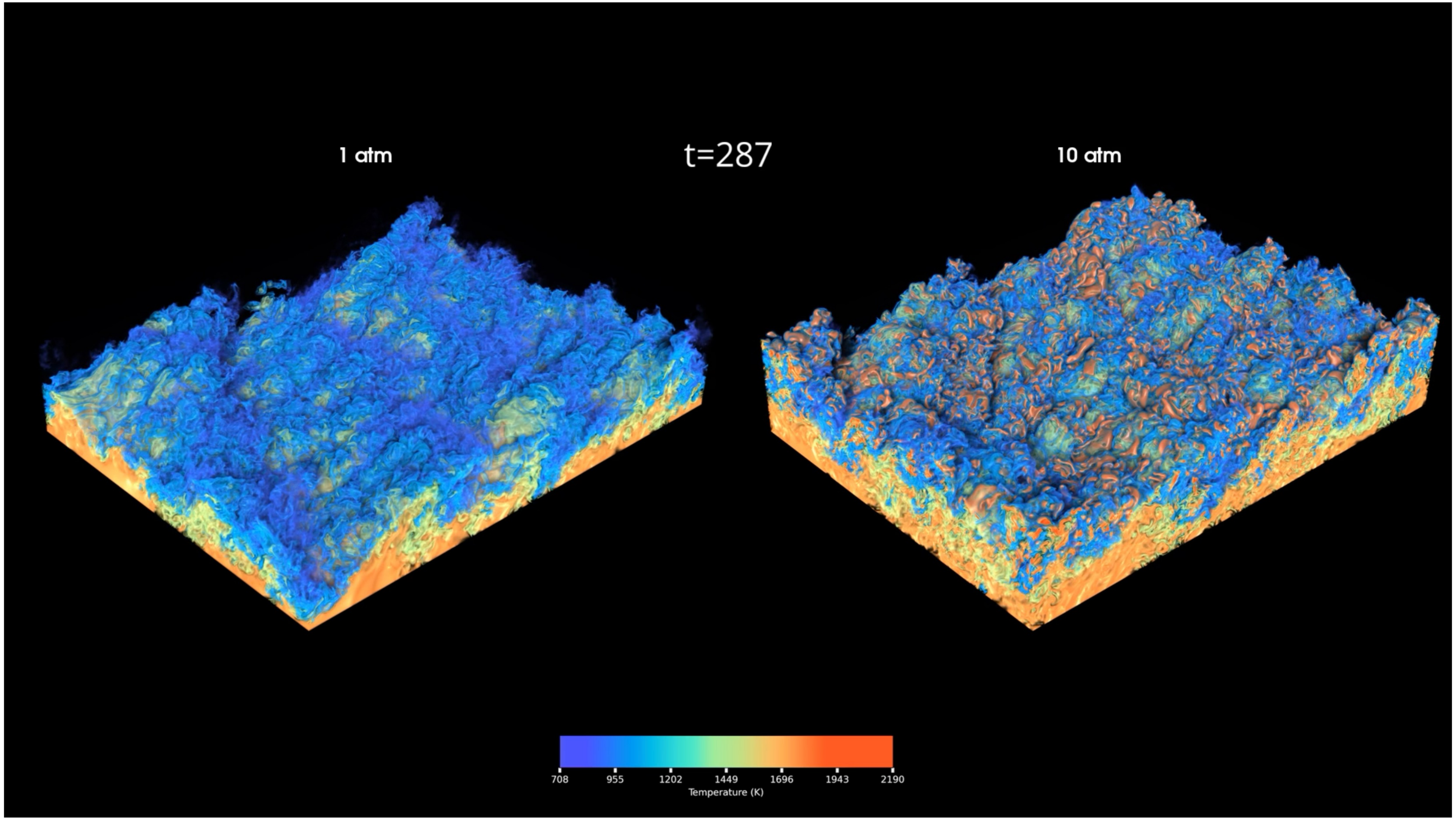
$$s_{c,\mathrm{fuel}} = I_0 s_l \sigma$$

I_0: stretch factor

Flame surface density

- Flames with same unstrained laminar flame properties can behave very differently under turbulent conditions
- DNS showed strong impact of hydrogen diffusion on the $NH_3/H_2/N_2$ flames

DNS LEAN $NH_3/H_2/N_2$ FLAMES – PRESSURE DEPENDENCE



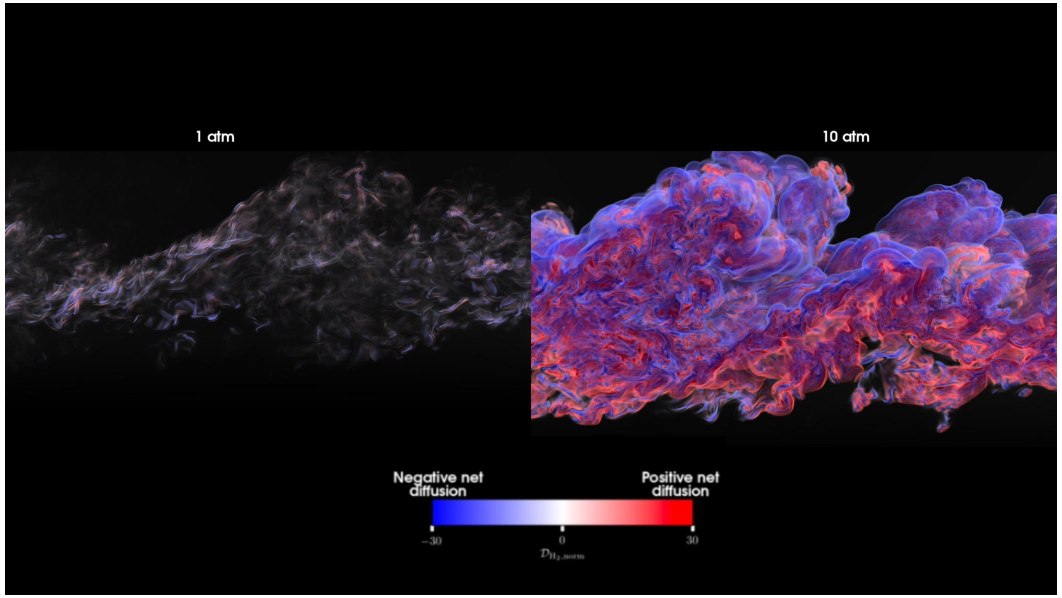
Mean flame propagation

NH3/H2/N2-air flames at ϕ=0.45 at 1 and 10 atm

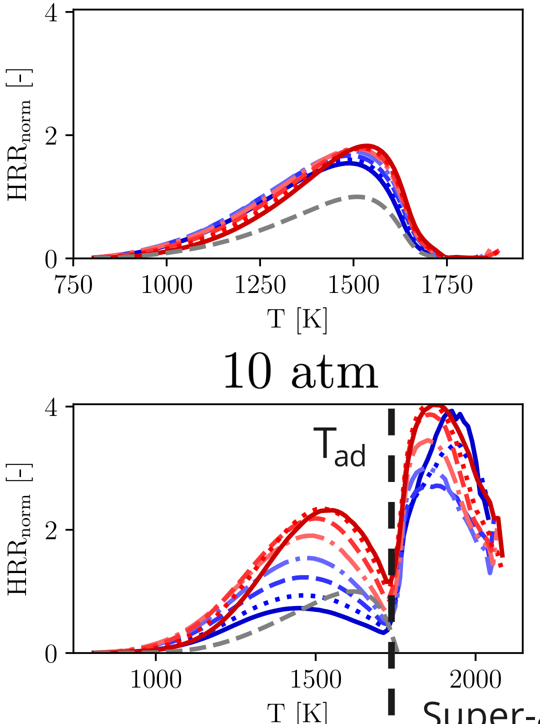
- Same turbulence-flame interaction properties based on unstrained laminar flame properties
- Orange regions 10 atm: super-adiabaticity

DNS LEAN $NH_3/H_2/N_2$ FLAMES – PRESSURE DEPENDENCE

H_2 diffusion rates

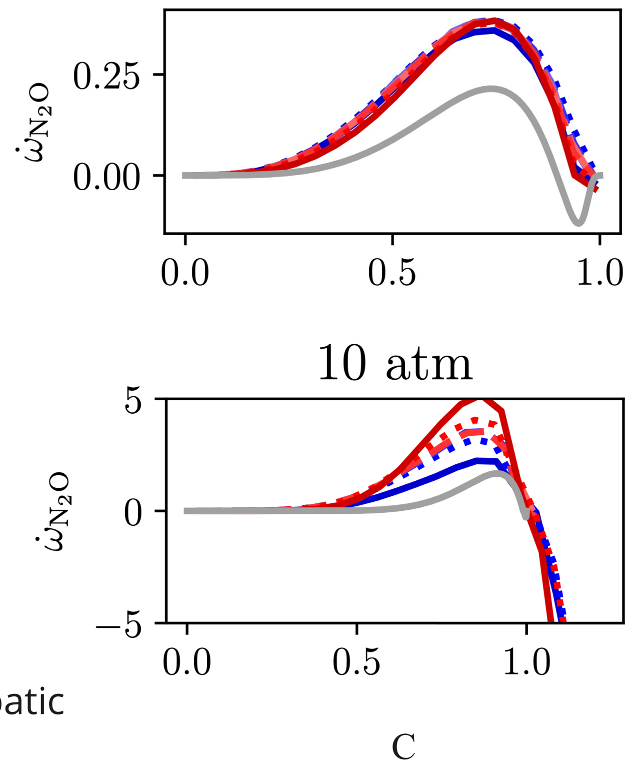


Curvature-dependent HRR



convex concave
(towards reactants)

Curvature-dependent emissions



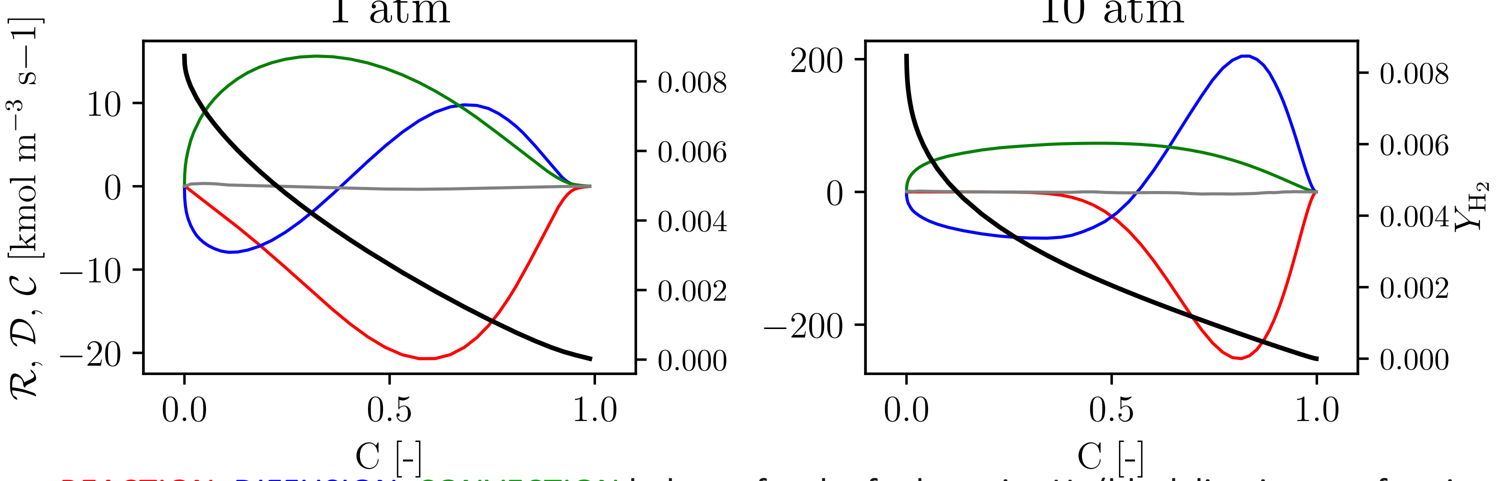
Chemical mechanism:
Jiang et al. (UCSD), 19 species

- Preferential diffusion effects are enhanced at elevated pressure
- HRR enhancement significantly amplified at higher pressure
- HRR & emission formation depend on small scales

Rieth et al., C&F, 2022; Rieth et al., PROCI, 2023.

SCALING OF LEAN HYDROGEN-AIR FLAMES

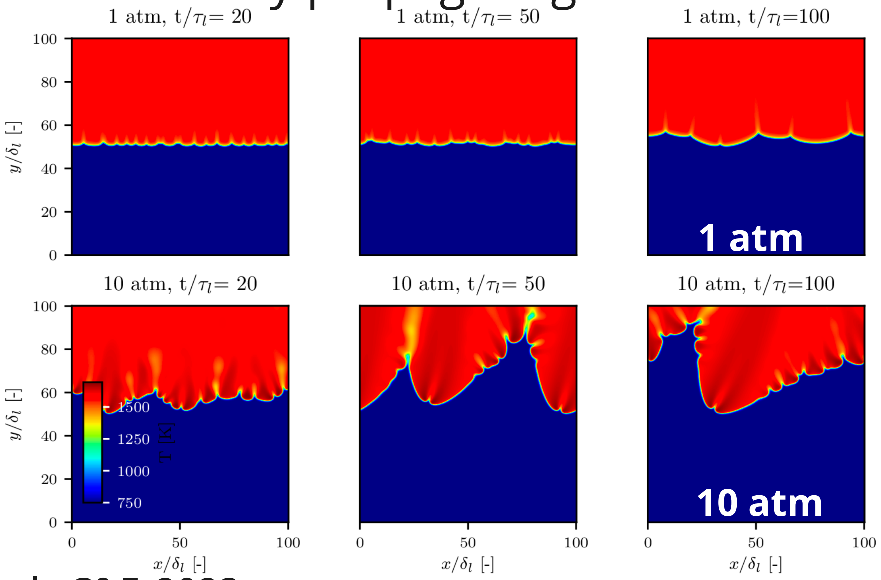
Laminar unperturbed flames



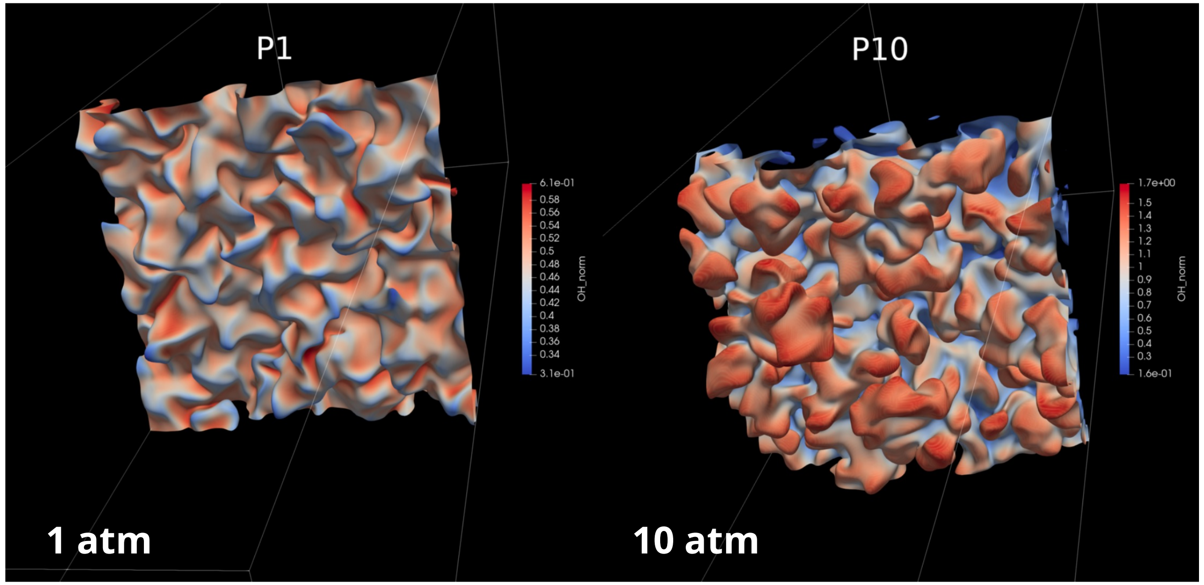
REACTION, DIFFUSION, CONVECTION balance for the fuel species H_2 (black line is mass fraction)

- Laminar 10 atm flame becomes 'weaker' through amplified chain-terminating three-body reactions (mainly $H+O_2+M=HO_2+M$)
- Fuel supply in reaction zone more dependent on diffusion as pressure increases

Freely propagating flames



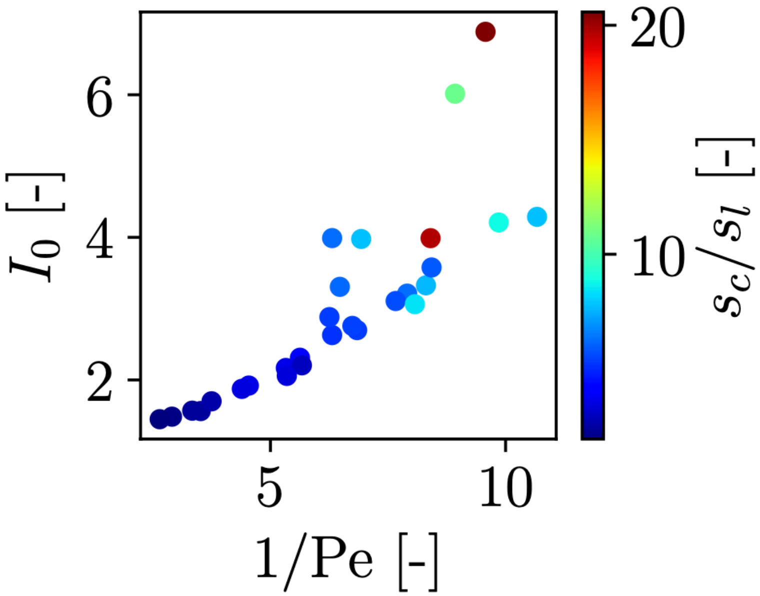
Flames in isotropic turbulence

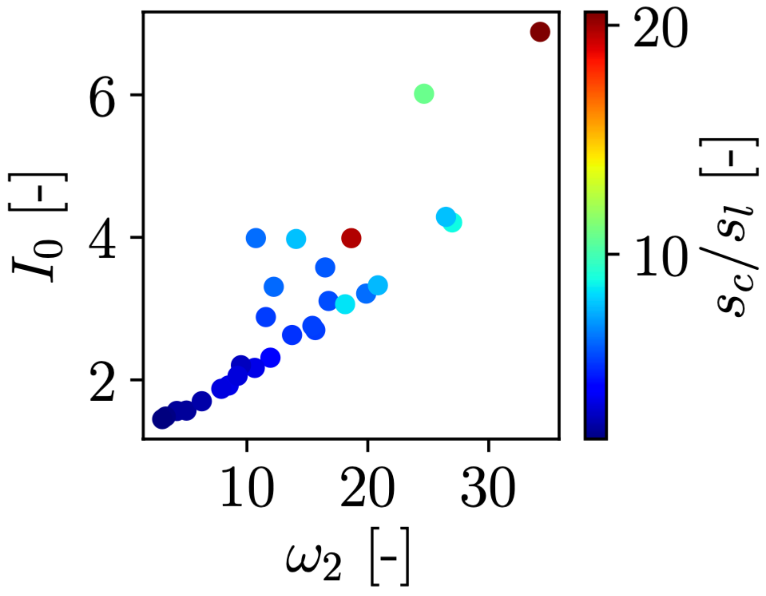


Rieth et al., C&F, 2023.

SCALING OF LEAN HYDROGEN-AIR FLAMES

Freely propagating flames

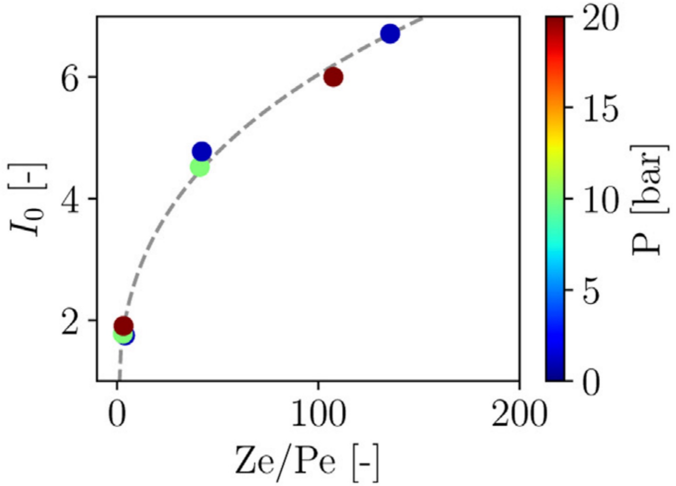




$$\omega = \omega_{\mathrm{DL}} k \underbrace{-[B_1 + \mathrm{Ze}(\mathrm{Le}_{\mathrm{eff}} - 1) B_2 + \mathrm{Pr} B_3]}_{\omega_2}$$

$$\mathrm{Pe} = |\mathcal{C}_{\mathrm{H_2}}|_{\mathrm{1D,max}} / |\mathcal{D}_{\mathrm{H_2}}|_{\mathrm{1D,max}} = \frac{|\frac{\partial Y_{\mathrm{H_2}}}{\partial x} u|_{\mathrm{1D,max}}}{|\frac{1}{\rho}\frac{\partial}{\partial x}(\rho \frac{W_{\mathrm{H_2}}}{W_{\mathrm{m}}} D_{\mathrm{H_2}} \frac{\partial X_{\mathrm{H_2}}}{\partial x})|_{\mathrm{1D,max}}}$$

Flames in 2D 'turbulence'
(all with same TCI params)

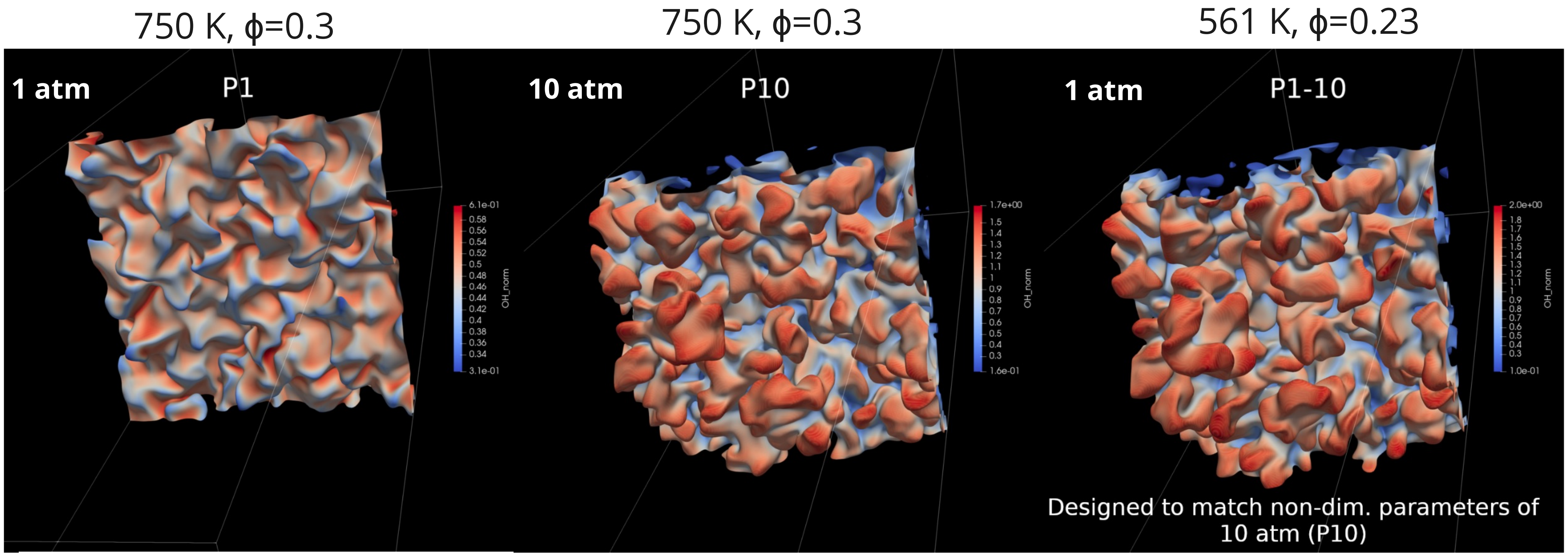


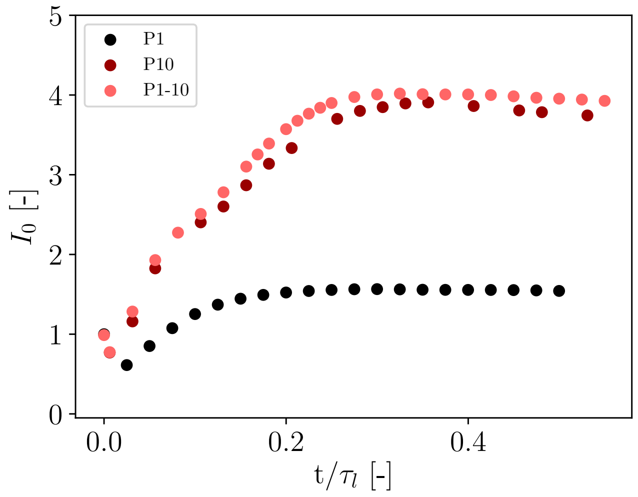
$$\mathrm{Ze} = 4\,(T_b - T_u)\,/\,(T_b - T_0)$$

- Howarth & Aspden (C&F, 2021) used ω_2 (dispersion model by Matalon et al., 2003) to predict burning rate enhancement I_0
- Proposed Pe works similarly, is very easy to compute from 1D unperturbed flame

Rieth et al., C&F, 2023.

SCALING OF LEAN HYDROGEN-AIR FLAMES

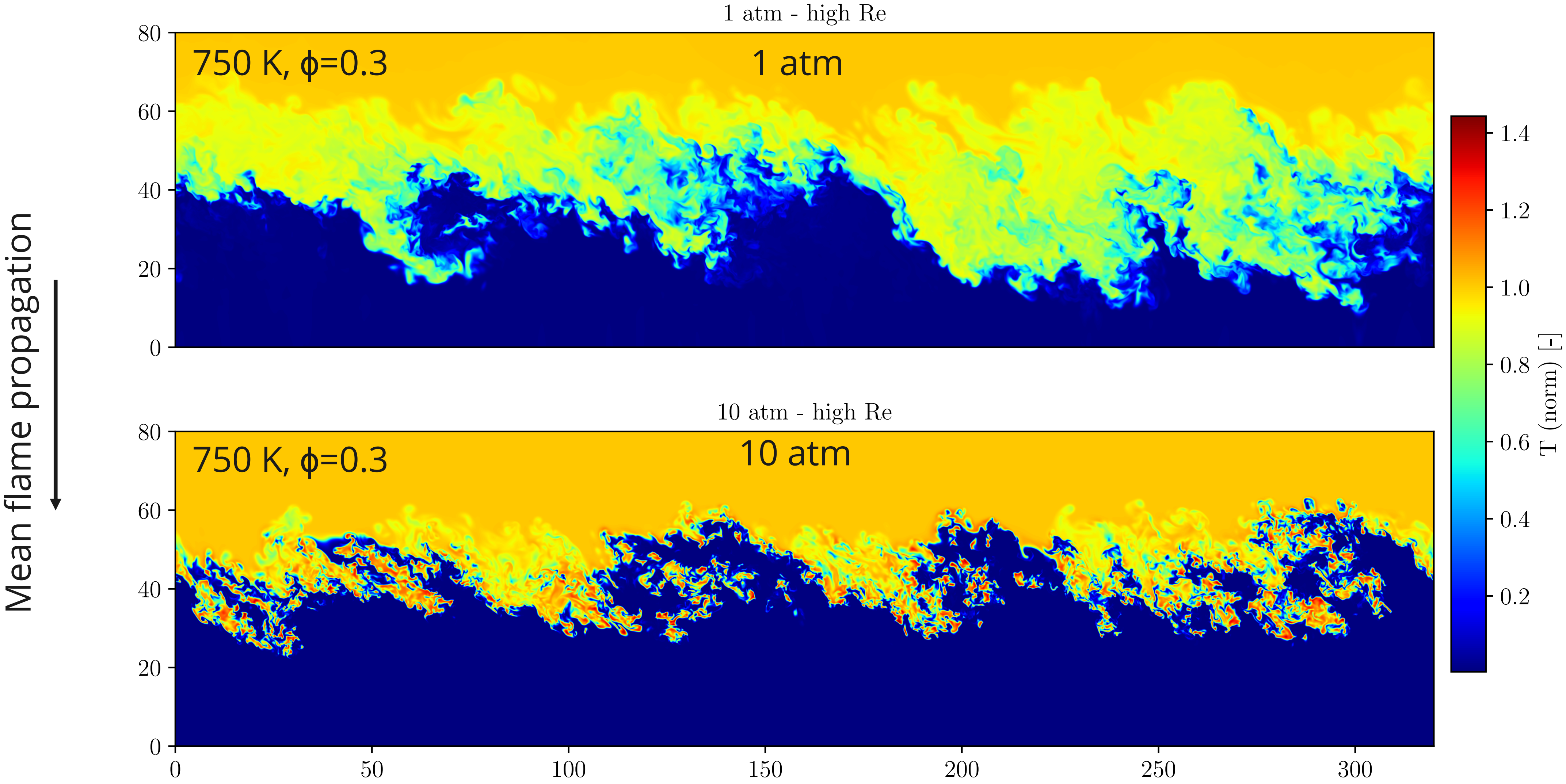




- 'Pressure effect' is not unique to pressure → same flame response can be evoked by changing unburned gas temperature and equivalence ratio
- Allows study of thermo-diffusive effects at atmospheric pressure – <u>also experimentally</u>

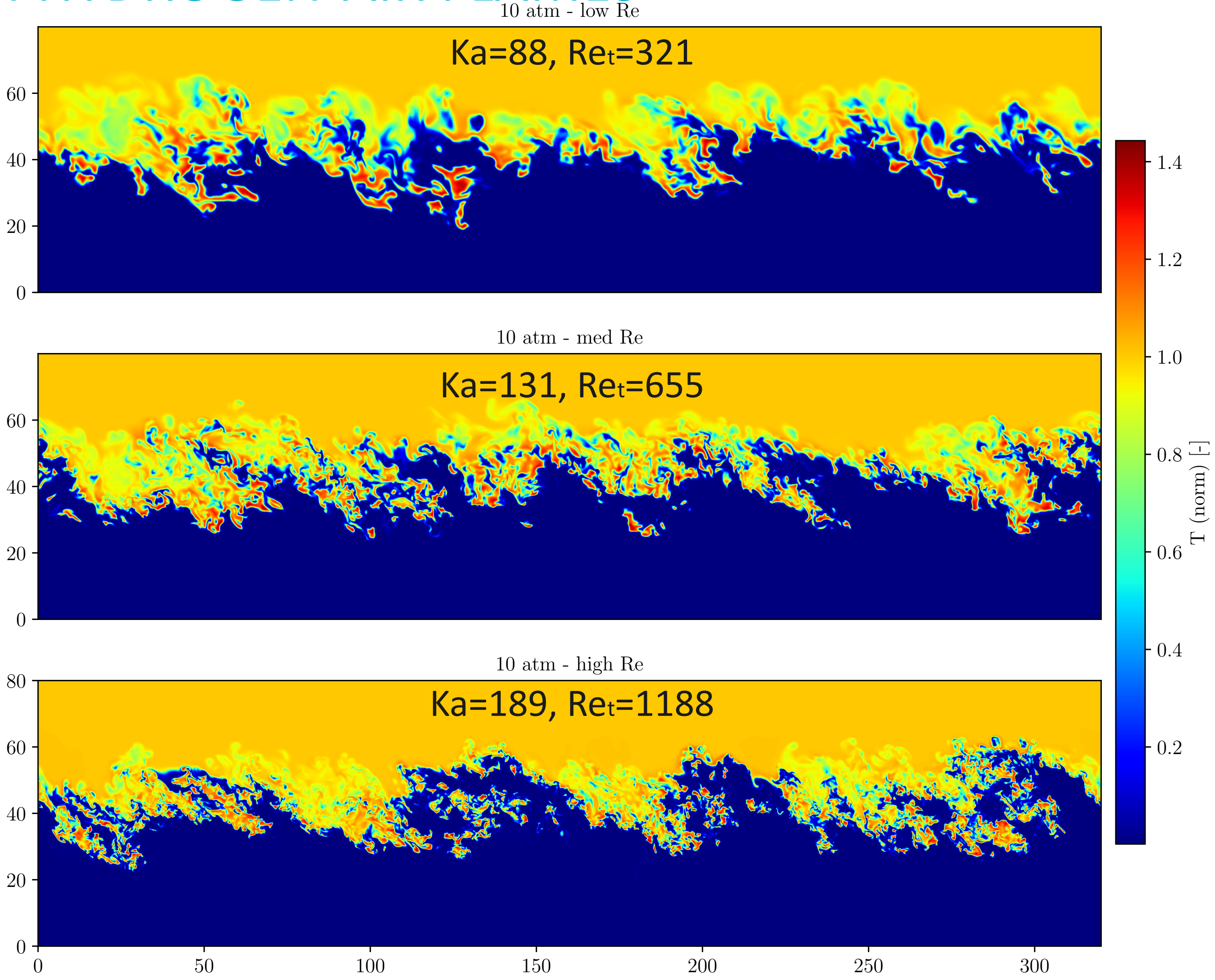
Rieth et al., C&F, 2023.

SCALING OF LEAN HYDROGEN-AIR FLAMES



- Lean H_2-air flames at high turbulence intensity 1 vs 10 atm
- Qualitatively similar to lean lean NH_3/H_2/N_2-air flames

SCALING OF LEAN HYDROGEN-AIR FLAMES

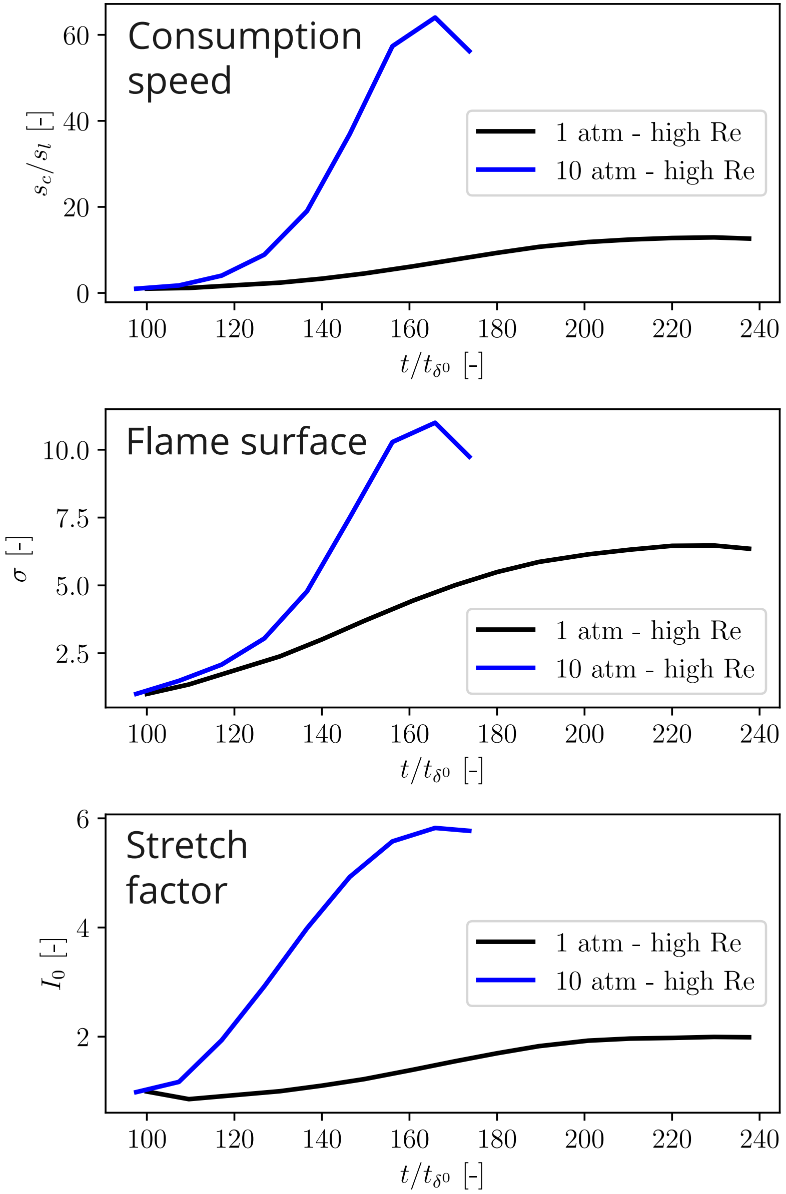


- Turbulence intensity clearly impacts flame surface area – how about burning rates?

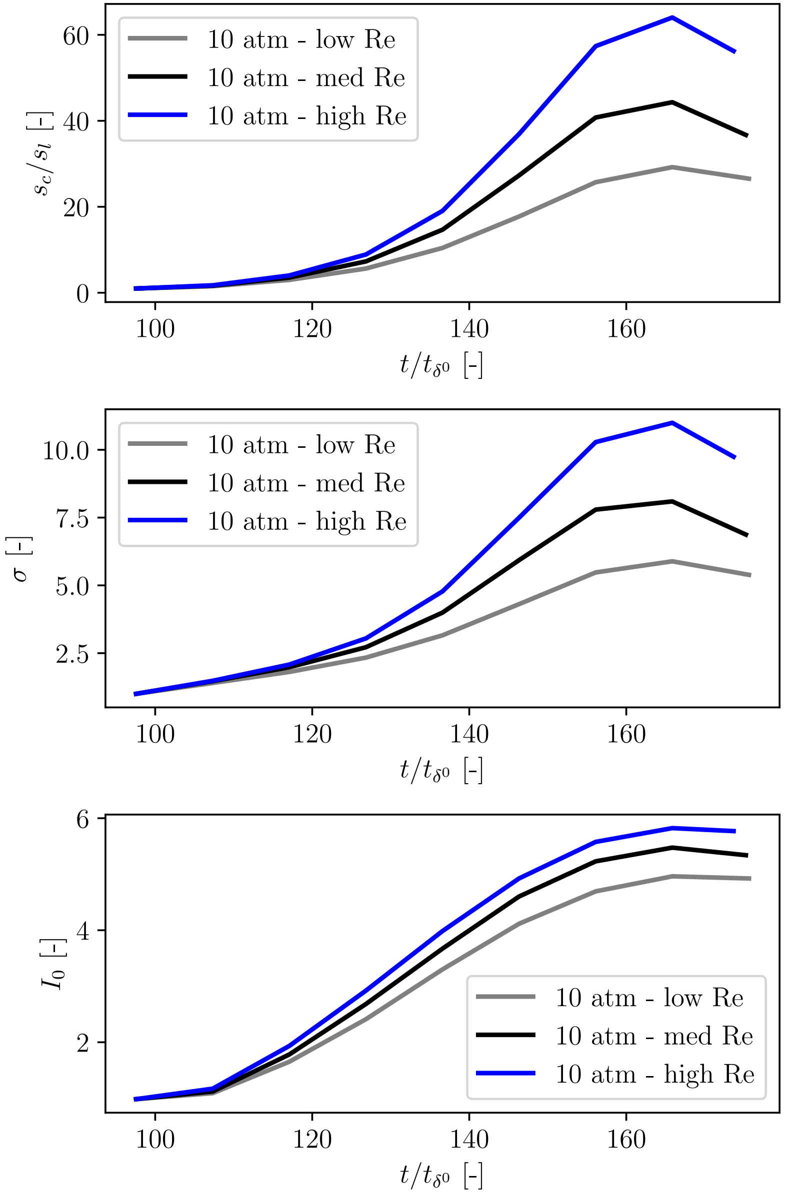
SCALING OF LEAN HYDROGEN-AIR FLAMES

Significant burning enhancement with pressure

Pressure impact



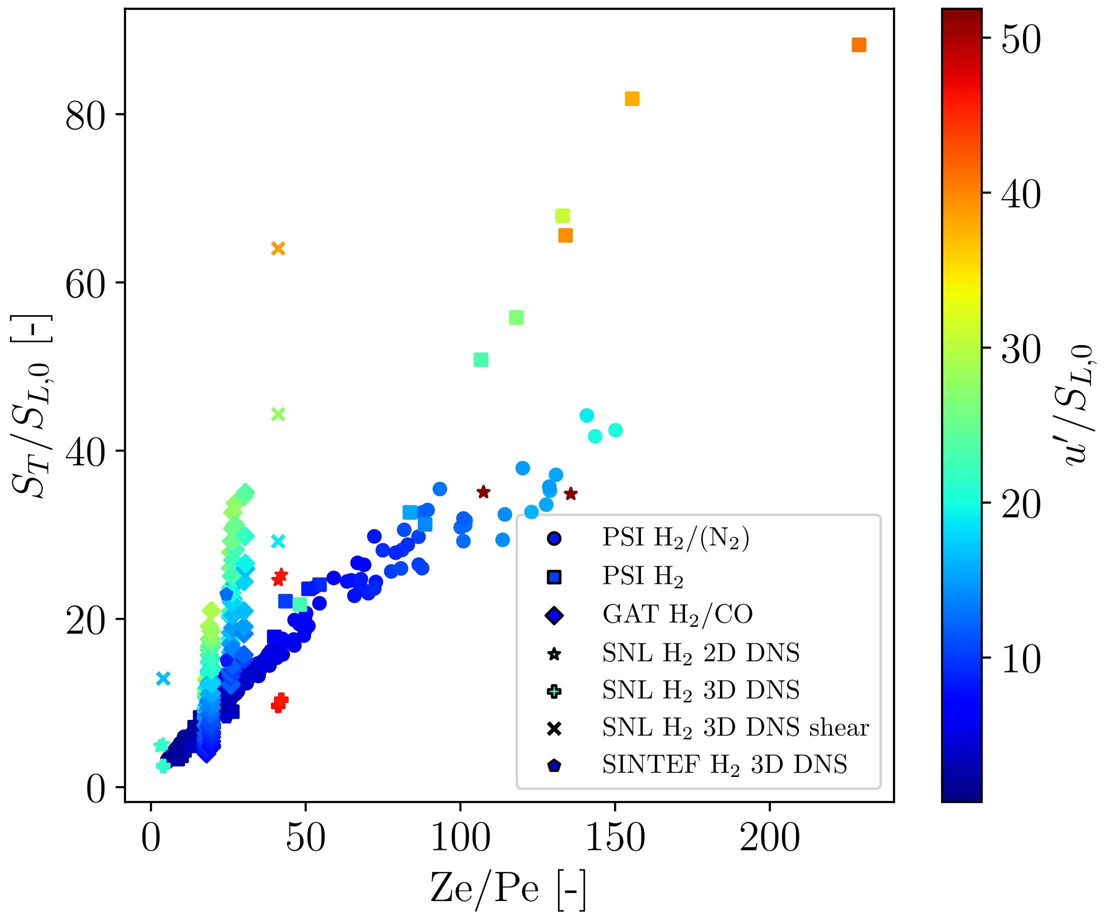
Turbulence impact

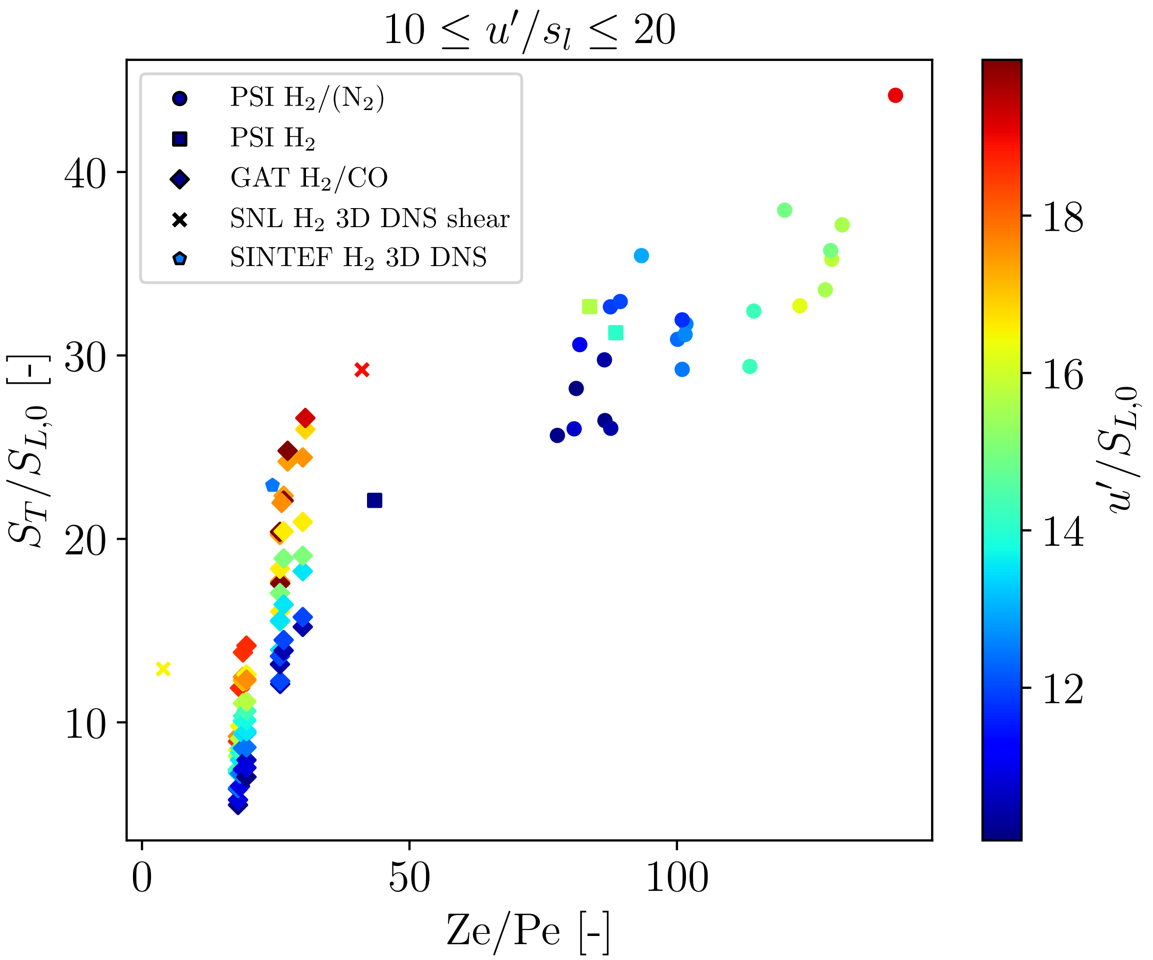


Burning enhancement with turbulence intensity – but to lesser extent on I_0

*For CH_4 flames it is a lot easier to extrapolate from atmospheric to higher pressures because I_0 does not change

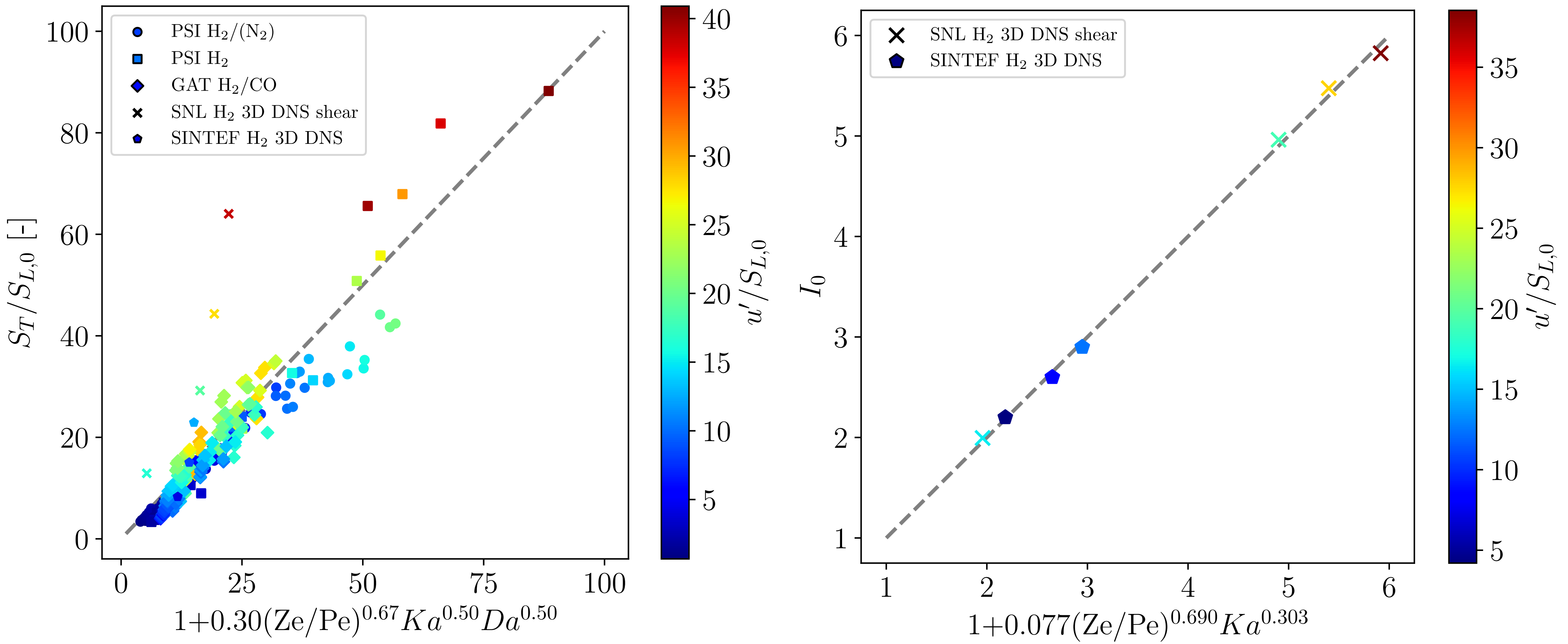
SCALING OF LEAN HYDROGEN-AIR FLAMES





- Combined DNS and experimental data shows scatter in S_T/S_l through impact of u'/S_l

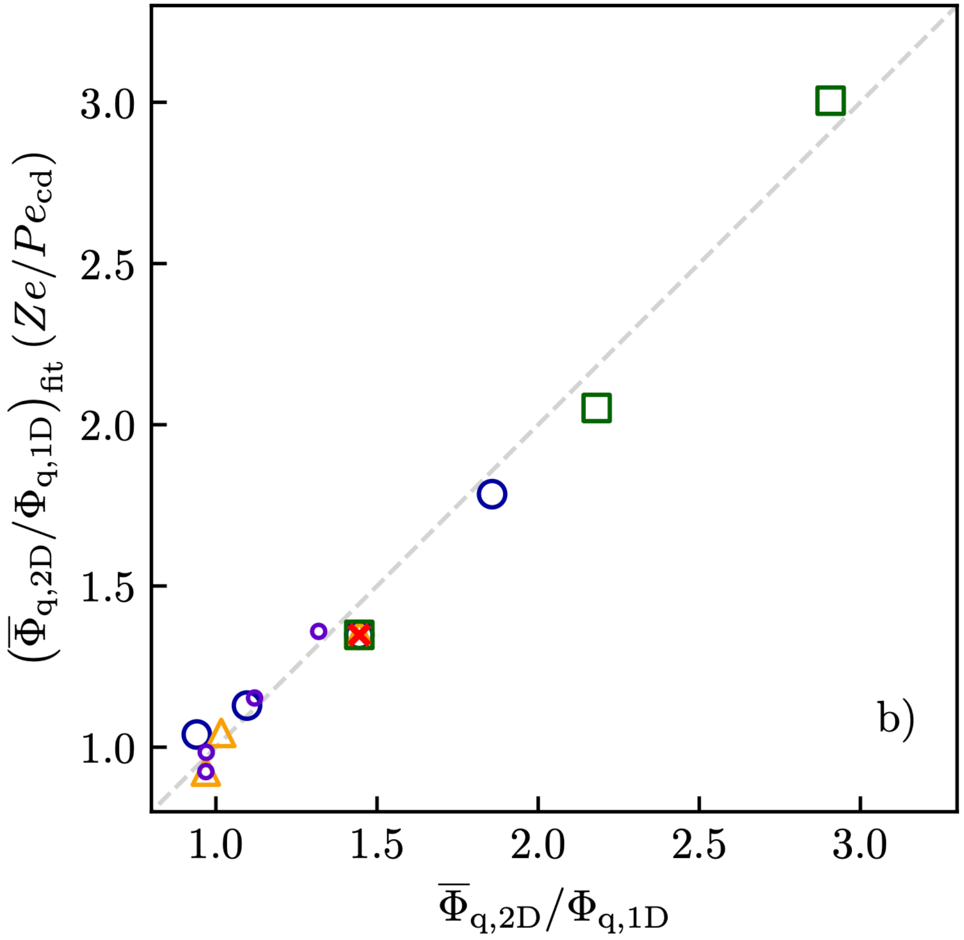
SCALING OF LEAN HYDROGEN-AIR FLAMES

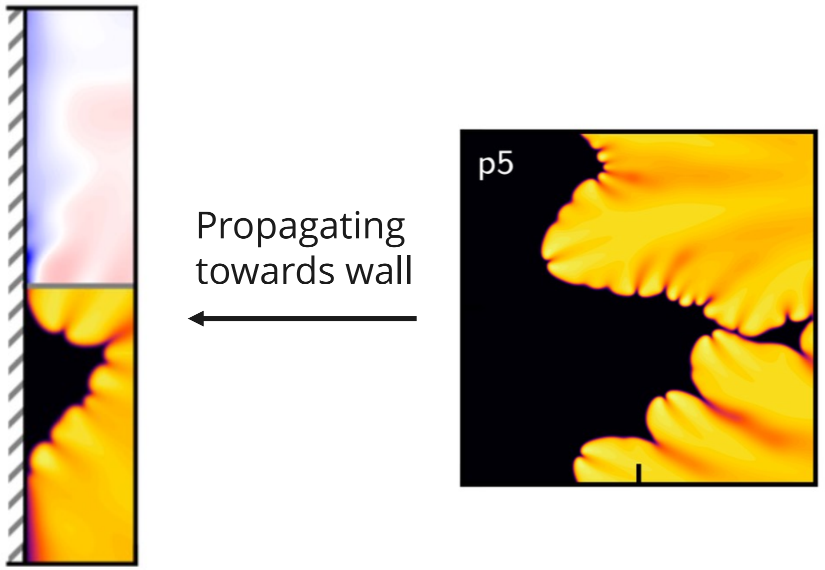


- Derived scaling taking into account turbulence parameters works quite well

$$I_0 = s_{c,\text{fuel}}/(s_l \sigma)$$

SCALING OF LEAN HYDROGEN-AIR FLAMES IN OTHER WORK





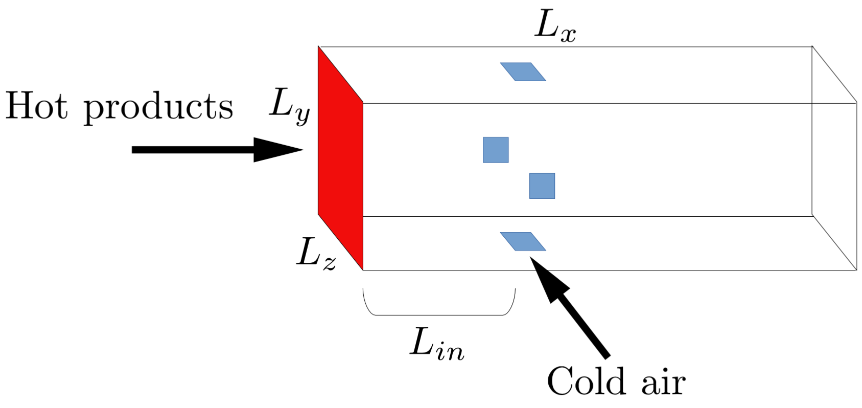
Work by TU Darmstadt:

- Pe/Ze was used to build a model for mean quenching wall heat flux
- Obtained very good agreement between modeled and simulated heat flux

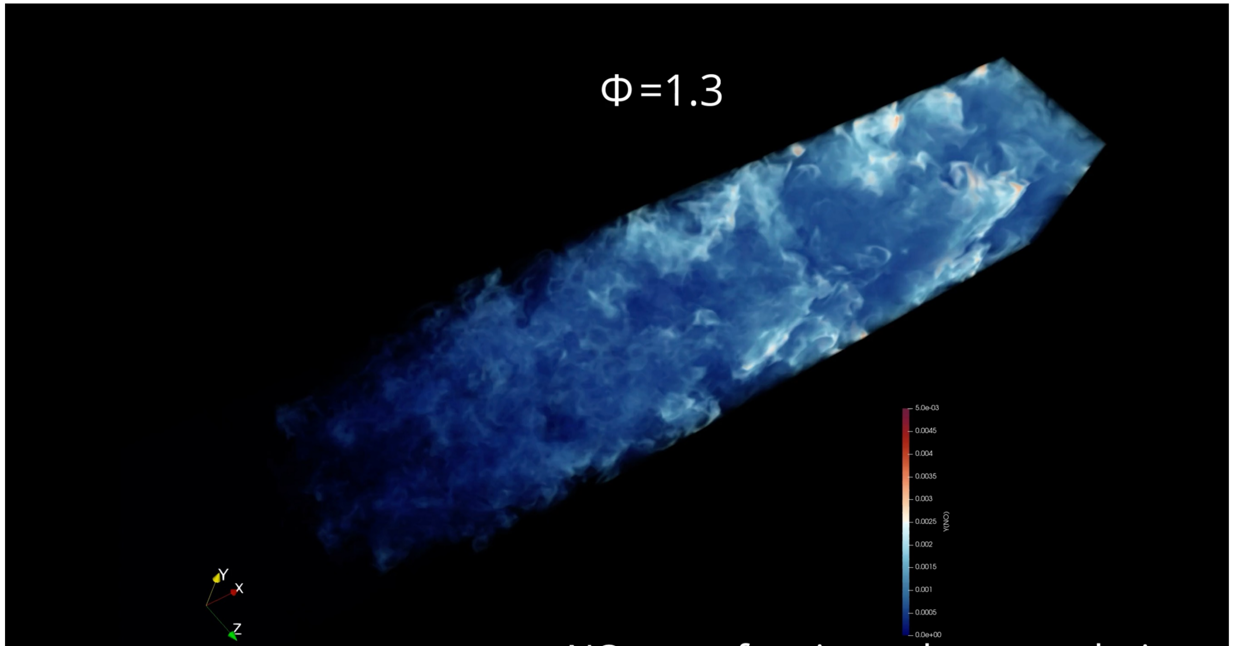
Schneider et al., arxiv, 2024.

STAGED AMMONIA COMBUSTION

STAGED AMMONIA COMBUSTION



Temperature volume rendering



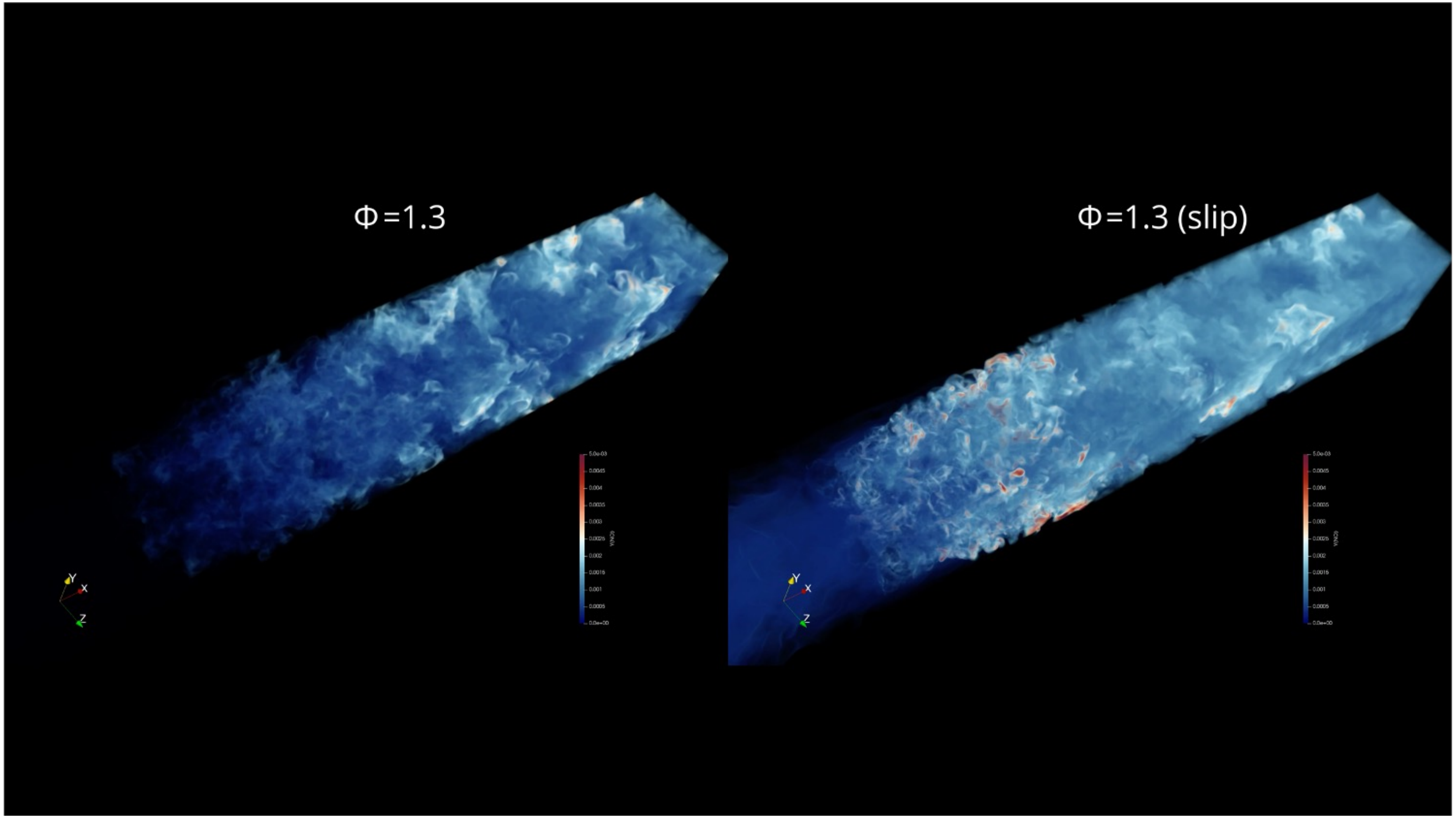
NO mass fraction volume rendering

- 2^{nd} stage of a staged combustor setup
- 1^{st} stage: rich premixed ammonia(/hydrogen) air flame
- 2^{nd} stage: pure air injection
- 25 atm
- Cross-flow: products from first stage
- Parameters derived from LES of actual gas turbine (but downscaled)
- 30 ms residence time 2^{nd} stage

Rieth et al., PROCI, 2024.

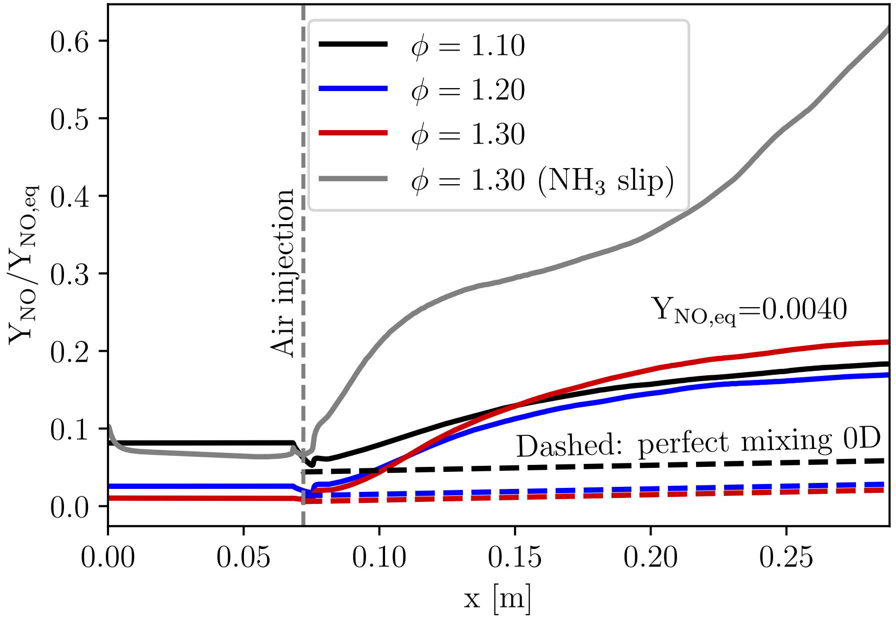
STAGED AMMONIA COMBUSTION

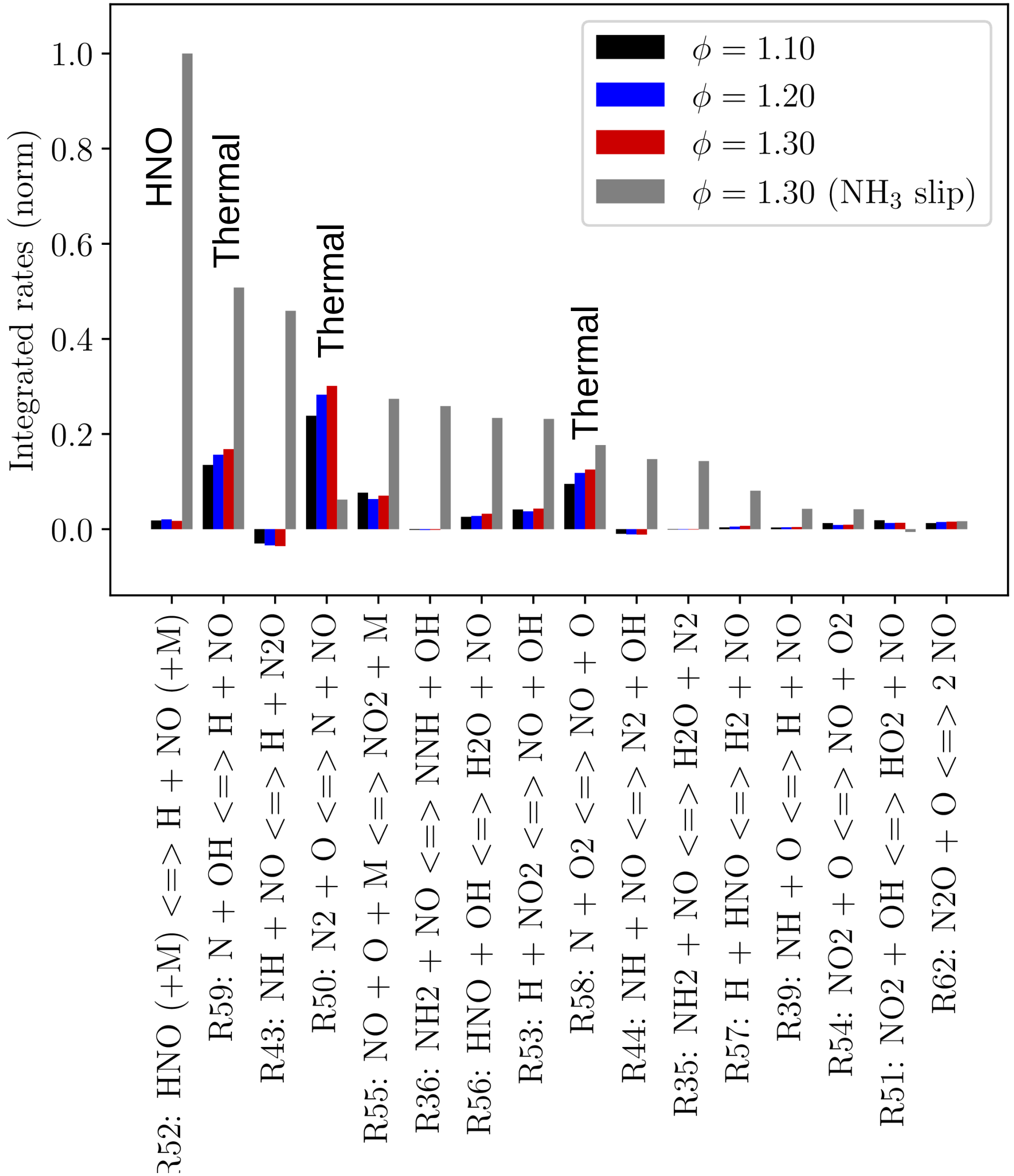
NO mass fraction volume rendering



- Unburned ammonia slip at the walls leads to increased NO production

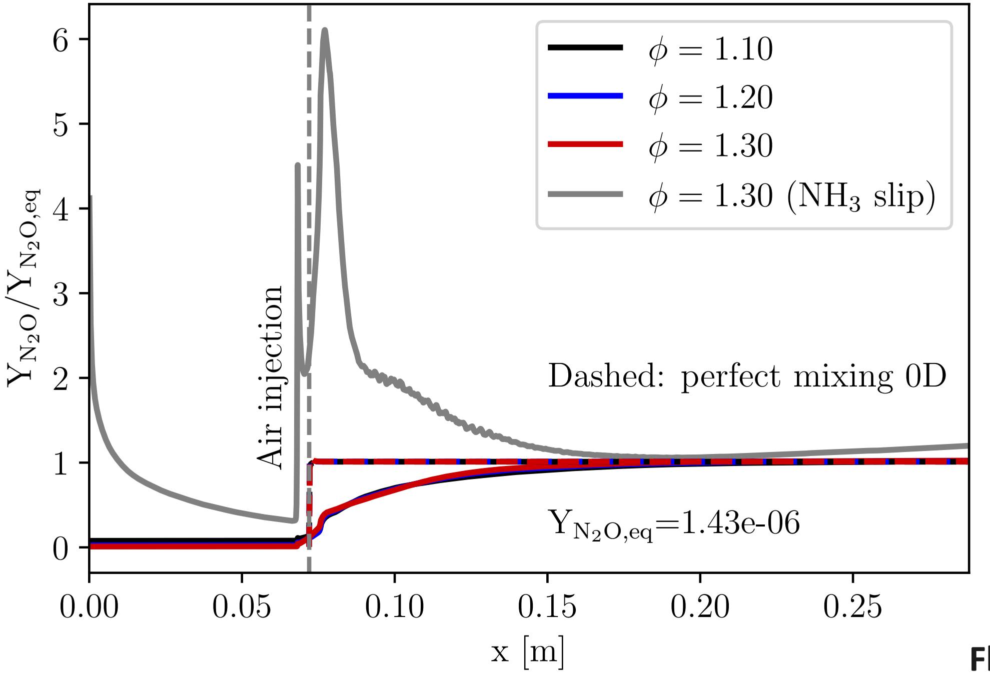
STAGED AMMONIA COMBUSTION

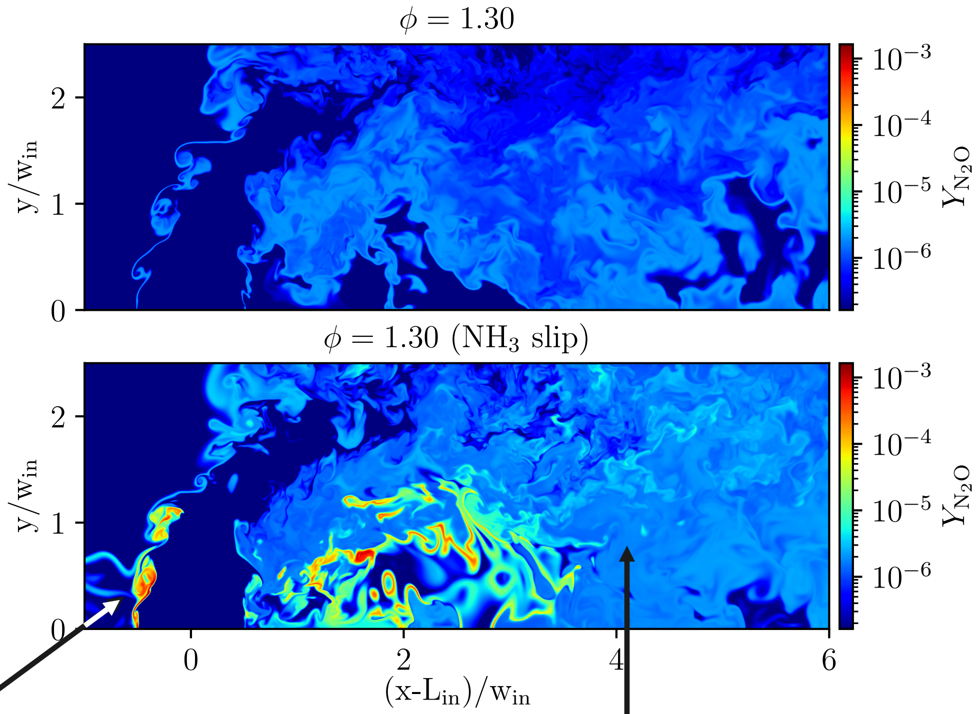




- Richer 1st stage: lower cross-flow NO, but faster NO production post air injection
- Ammonia slip significantly amplifies NO production (in flame zone but also downstream)

STAGED AMMONIA COMBUSTION





Flame
Prod: $NH+NO=H+N_2O$
Consumption: $H+N_2O=N_2+OH$

Lean side
$N_2O+(M)=N_2+O+(M)$

- Production of N_2O is very different to NO
- Ammonia slip has an impact on flame N_2O, but not much on downstream N_2O

DNS FOR AMMONIA/HYDROGEN FLAMES – CHALLENGES

Physics/modeling

- How to obtain a reliable, universal scaling for hydrogen-enriched flames (including blends) across a large spectrum of conditions to improve models? Need more experimental and DNS data

Simulation capabilities

- Capabilities have made huge strides in the past decade, DNS of laboratory scale experiments is now feasible – elevated pressure is still a challenge

Chemical mechanisms

- There has been a lot of work in ammonia mechanisms in recent years – what is the impact on DNS results? What is tractable?

Computing hardware

- Hardware has moved away from traditional double precision CPU FLOPS (lower precision computing for AI) – algorithms need to be adapted to take full advantage of hardware

DNS data impact

- How can we make DNS data more impactful? Is there a way to distill data in a way that is more useful for applications? How to fuse data from experiments and DNS?

Thank you for your attention!

The work at Sandia National Laboratories was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences.
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