



Large eddy simulations of turbulent jet flames at high pressures

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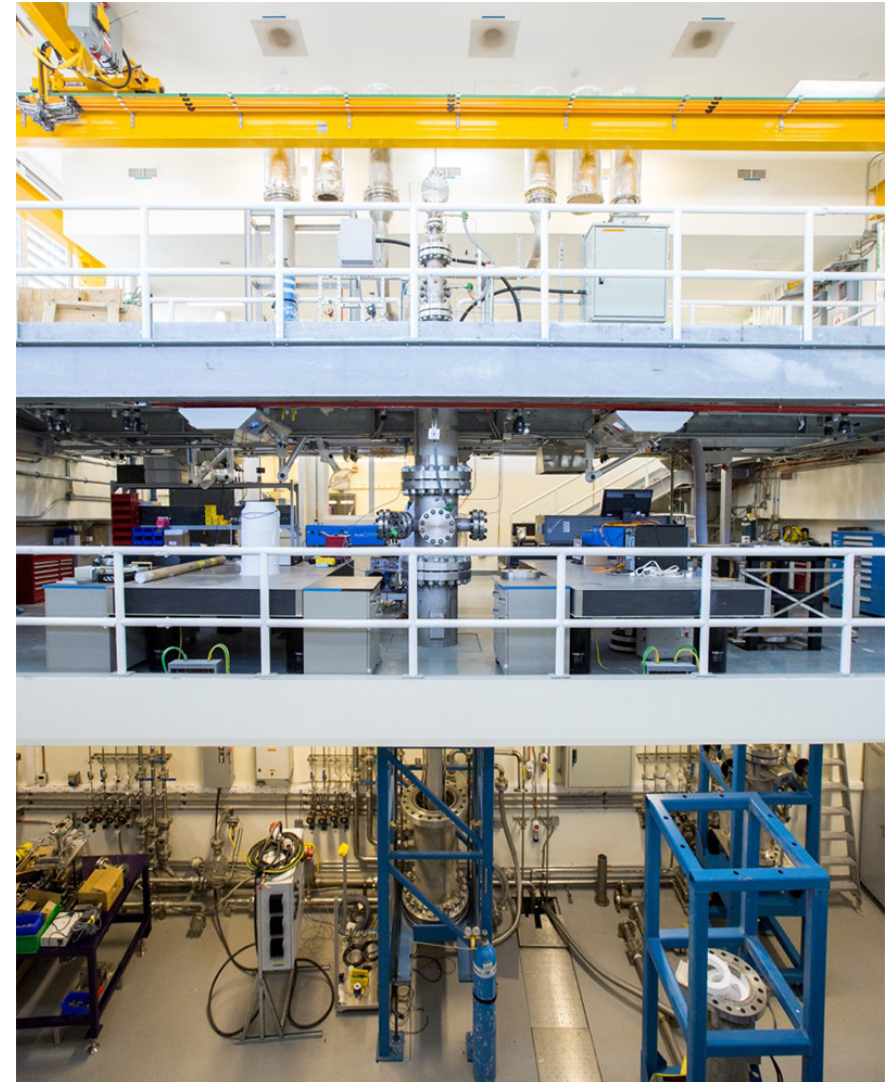
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Large eddy simulations (LES) of high pressure turbulent nonpremixed flames

- Simulation campaign aligned with the experimental effort in the Clean Combustion Research Center (CCRC) at KAUST
William Roberts, Gaetano Magnotti
Thibault Guiberti, Wesley Boyette
- CCRC has set up a high pressure combustion facility that can operate at up to 40 atm
- The simulations consider the experimental operation conditions and are aimed at cross-validation with the laser diagnostic measurements of various flame observables (PIV, LIF, LII)



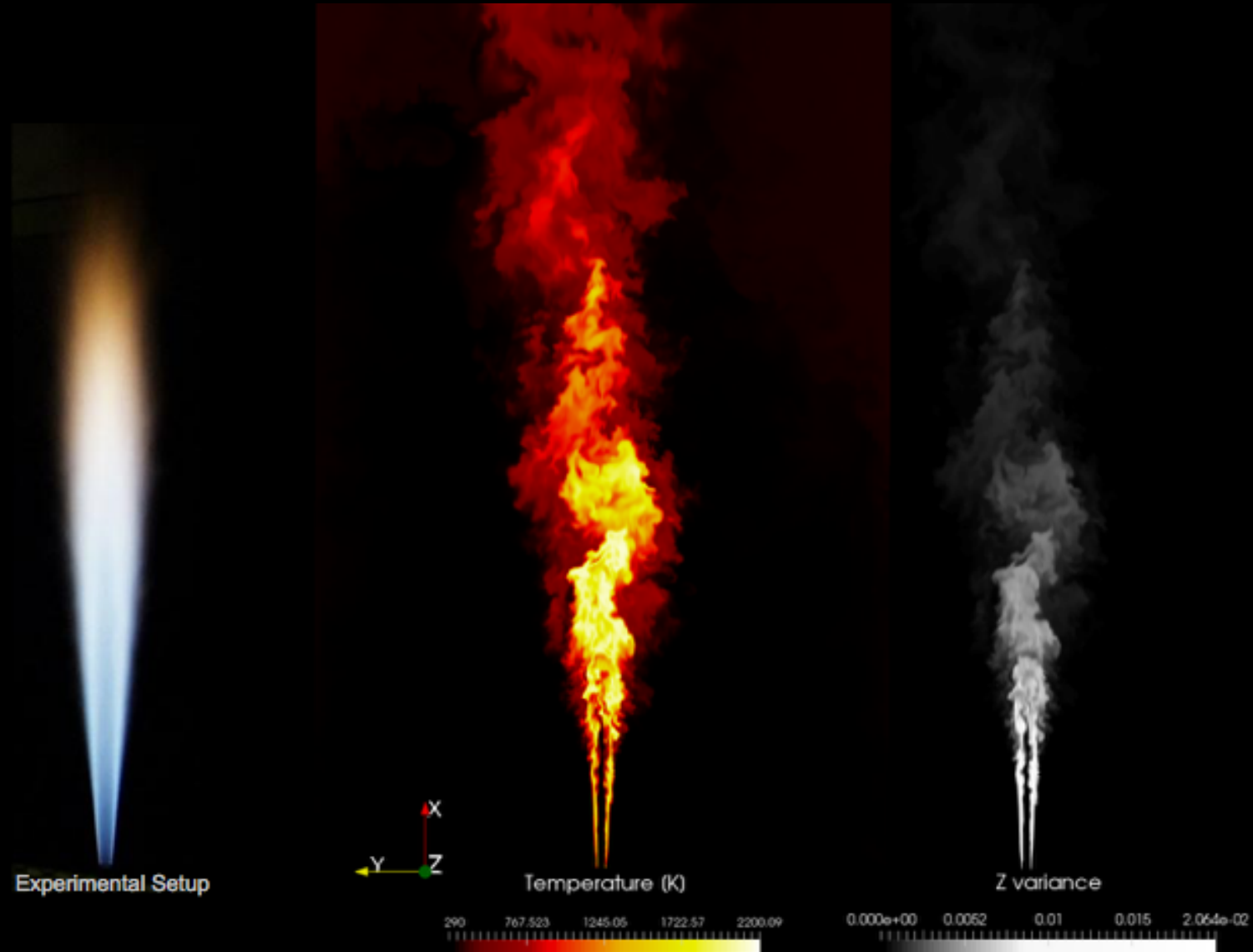
Outline and simulation strategy



- Numerical setup **validation** against Sandia flame A (syngas) experimental data at atmospheric pressure
- An *a priori* study on laminar counter-flow flames
- Assessment of flamelet assumption for high pressure syngas-air flames
- Two series of flames simulated from 1 to 10 atm (1, 2, 5, 10 atm)
 - Series A: **constant Reynolds** number ($Re=16700$)
 - Series B: **constant** inflow **velocity** ($U=84.7$ m/s)

Validation of the numerical setup (p=1atm)

Comparison with measurements of Sandia flame A



Baseline case - Sandia flame A

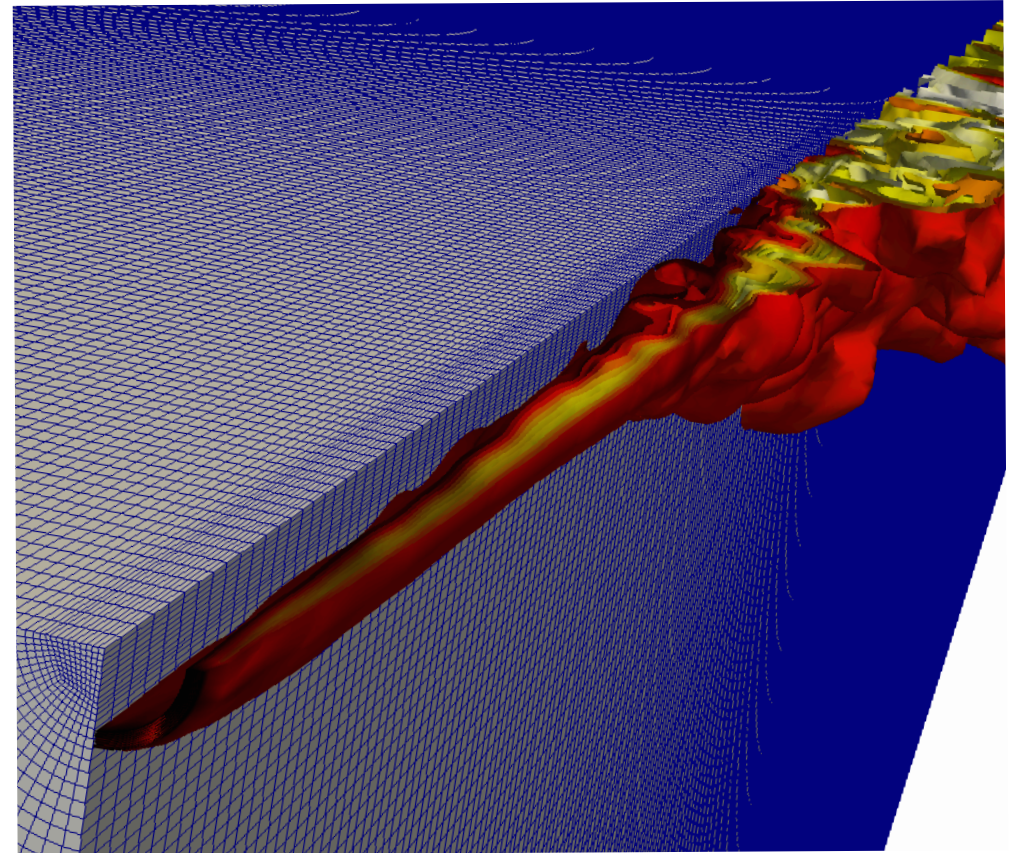


- Nonpremixed turbulent flame at $p = 1$ atm
- Fuel composition: 40% CO / 30% H₂ / 30% N₂
- Fuel jet velocity $U_{\text{jet}} = 76$ m/s, Reynolds number 16,700
- Fuel jet nozzle: ID 4.58 mm, OD 6.34 mm
- Oxidizer: air at $U_{\text{coflow}} = 0.75$ m/s
- Scalar measurements (Raman/Rayleigh/LIF for T & Species)
- Velocity measurements with LDV
- **Characterization of similar flames at higher pressures is being conducted at CCRC**

Sandia Flame-A (chn-A)

Large eddy simulation numerical setup

- Favre-filtered Navier-Stokes equations are solved using a **finite volume pressure-based** solver of **OpenFOAM**
 - **Steady laminar flamelet model (SLFM)** for modeling combustion
 - Large eddy simulations (LES) using **Smagorinsky** model for **subgrid stresses**
 - Transport equations for mixture fraction Z and its variance Z''
 - A presumed (**beta**) filtered density function (**FDF**) approach is employed to represent the subgrid-scale (SGS) turbulence-chemistry interaction
-
- Flamelet library for Y_α and T is constructed and parameterized in terms of χ and Z
 - Flamelet solution using **12 species and 33** reactions (Li et al., 2007)^[1]
 - **7M cells for a 3D** computational domain (R=169 mm, L=960 mm)



LES

Temperature field

Experiments

KAUST CCRC labs



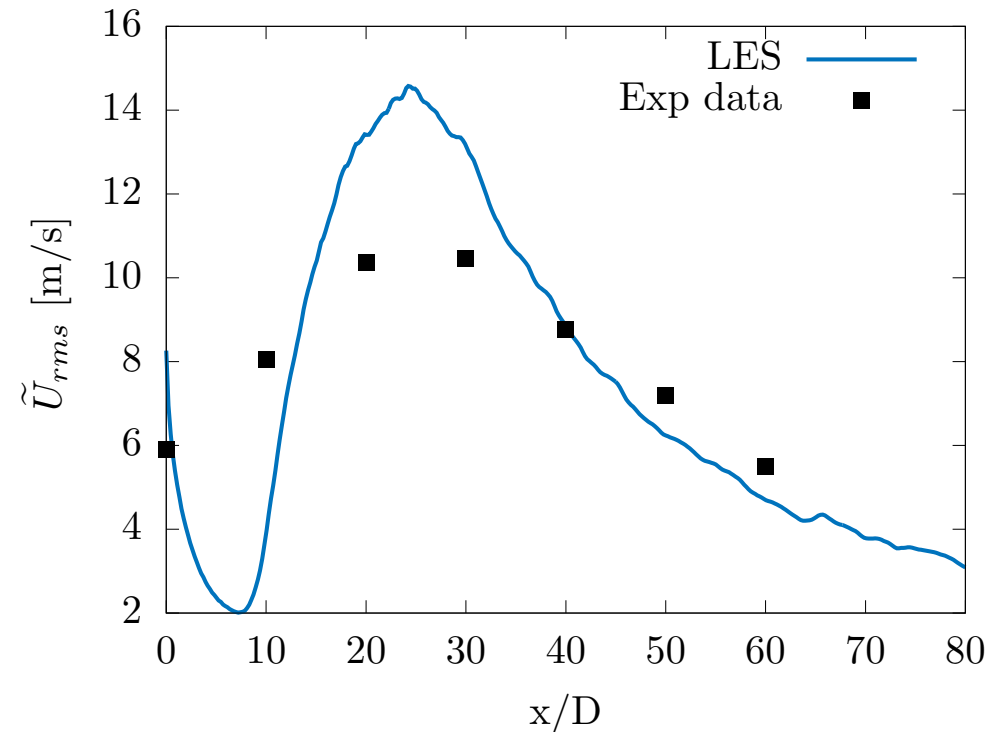
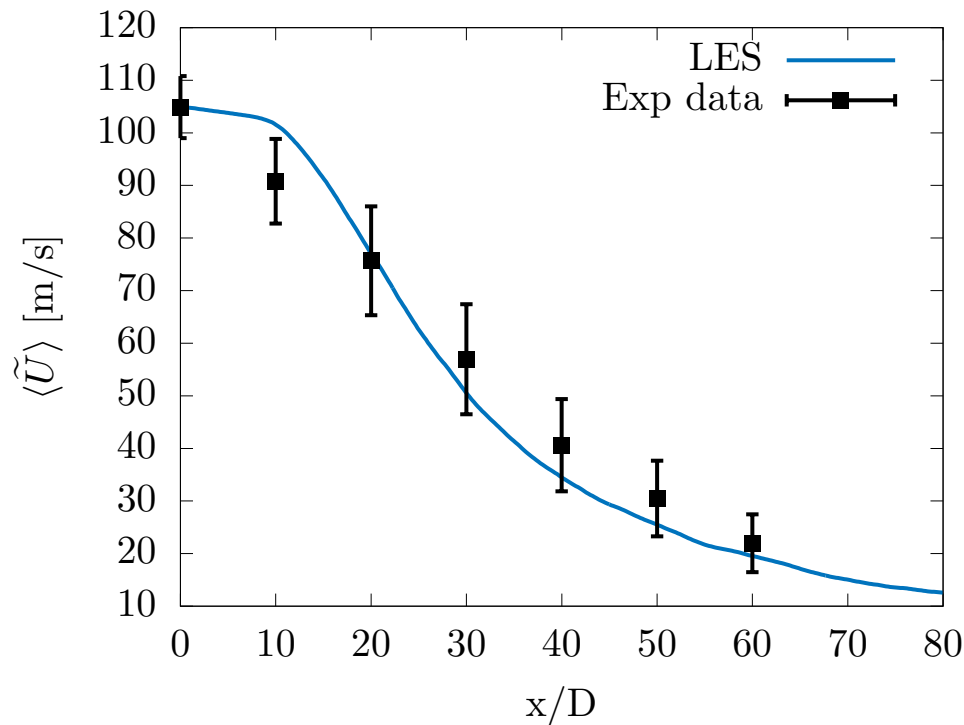
A first qualitative agreement is observed

Comparison with experimental results

Axial distribution of mean velocity



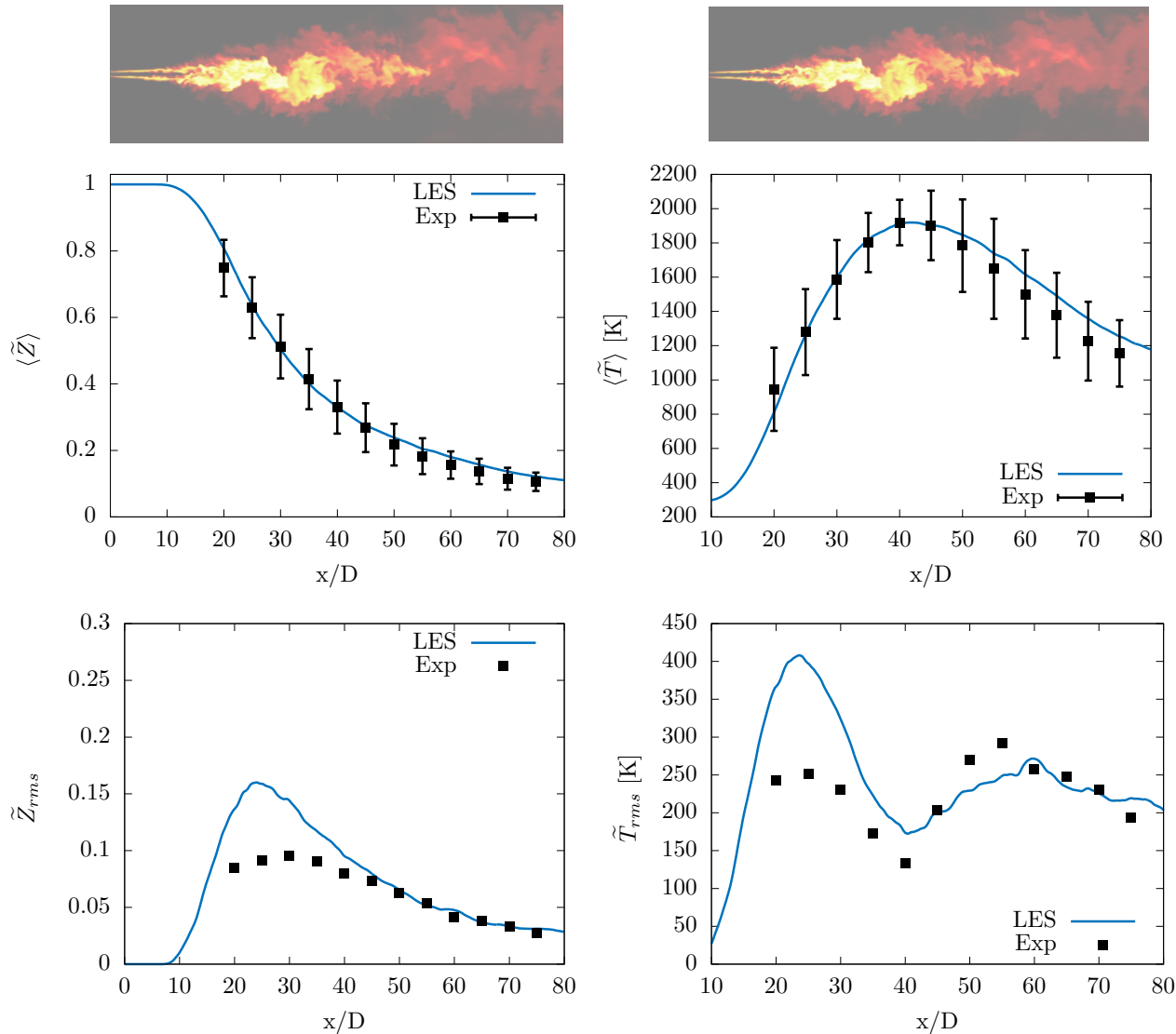
- Inflow: power law (fully developed turb. pipe)
- $Re = 16700$
- $U_{jet, mean} = 84.7 \text{ m/s}$
matching the experimental inflow profile ($U_{max} = 105.4 \text{ m/s}$)



- **Mean and rms of axial velocity** in satisfactory agreement with measurements

Comparison with experimental results

Axial distribution of mean temperature and mixture fraction



Agreement with measurements:

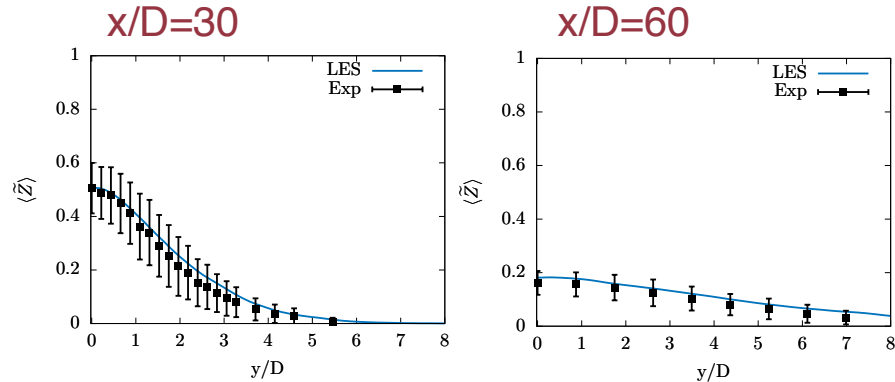
- mixture fraction **Z**
mean and rms

- temperature **T**
mean and rms

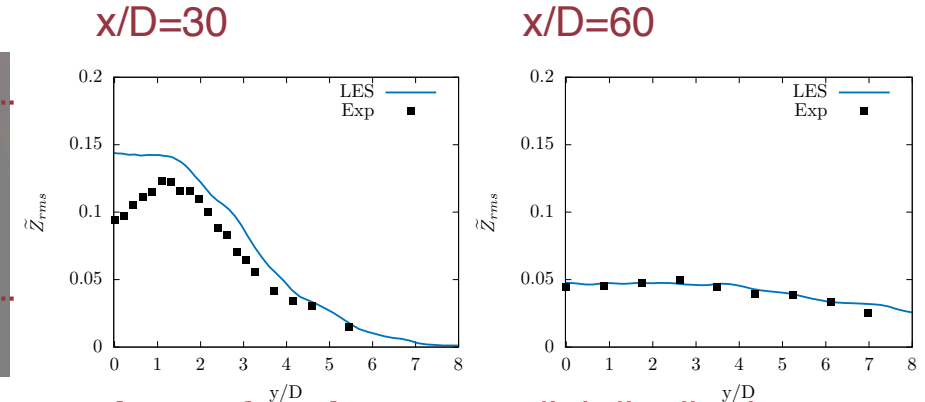
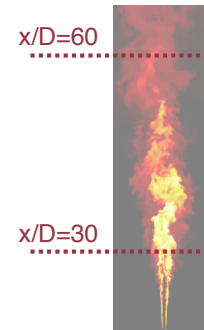
Comparison with experimental results

Radial distribution of mixture fraction and temperature

mixture fraction

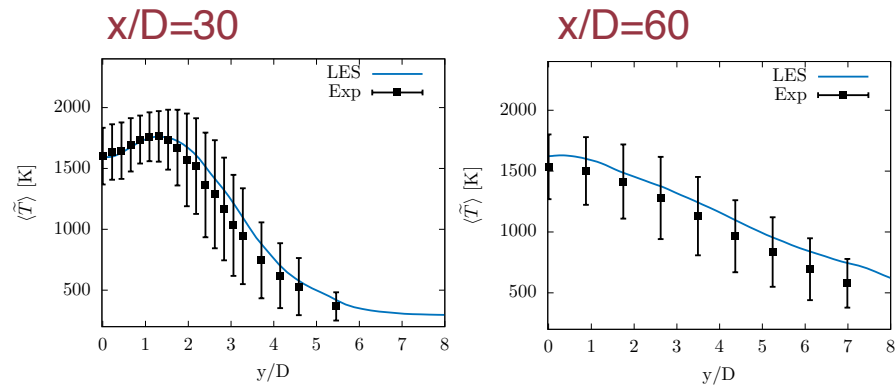


mixture fraction mean radial distribution

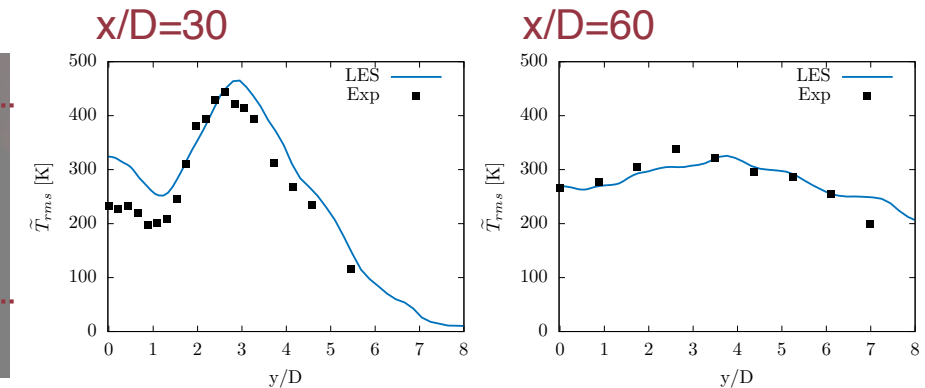
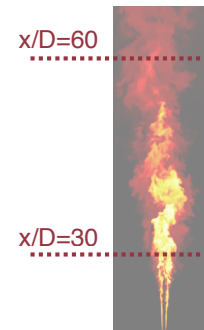


mixture fraction rms radial distribution

temperature



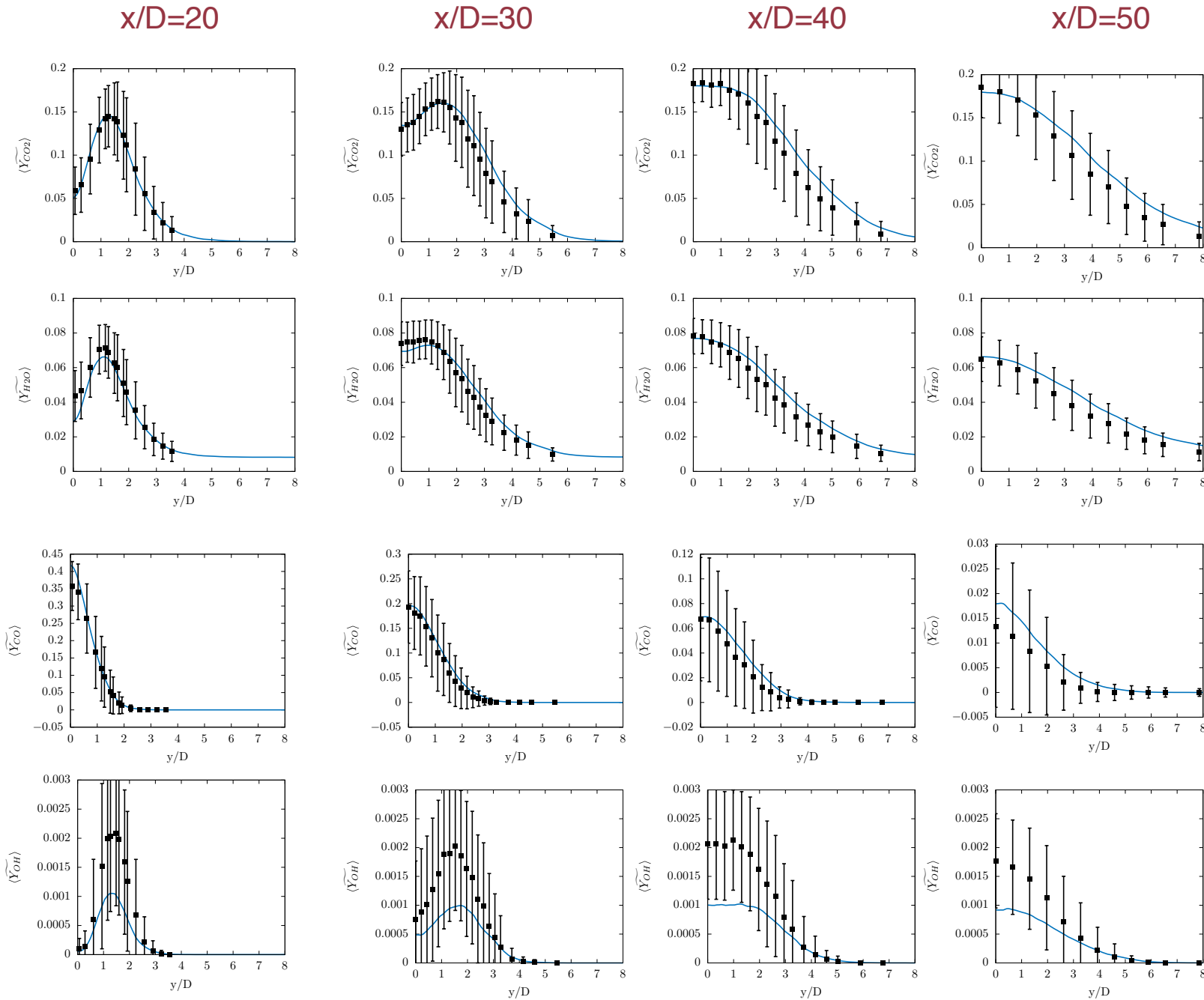
temperature mean radial distribution



temperature rms radial distribution

Comparison with experimental results

Radial distribution of species



CO₂

H₂O

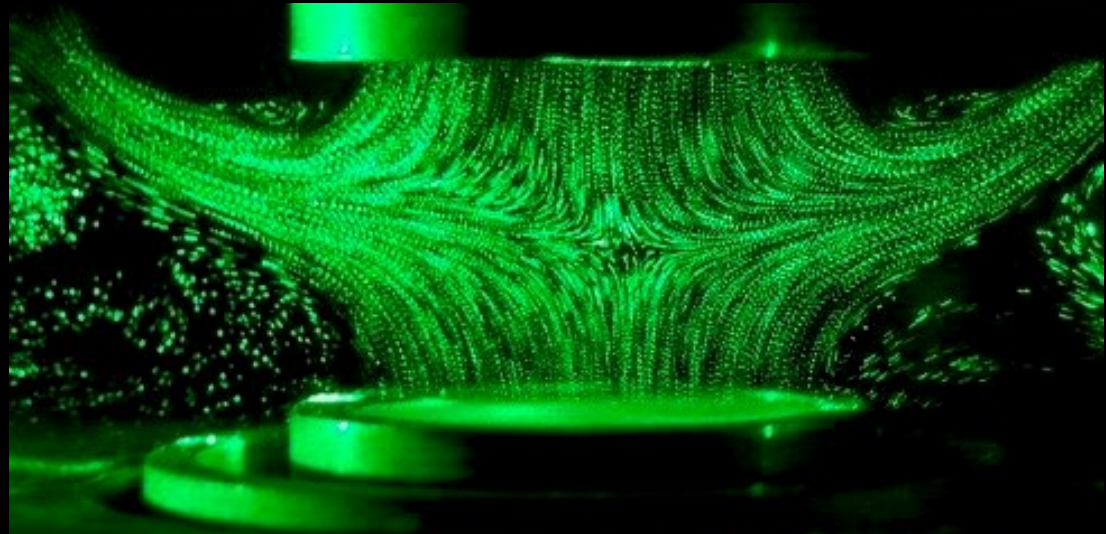
CO

OH

- major species
Good agreement

- OH
Slight discrepancy

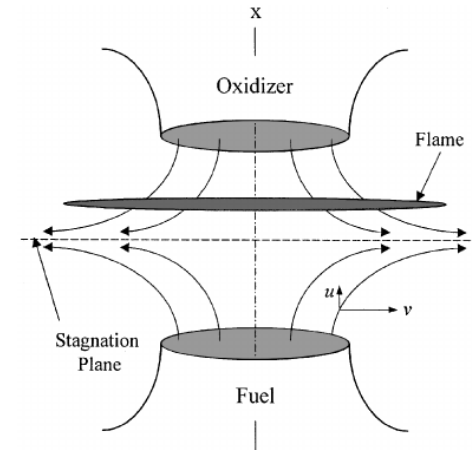
Effects of pressure on the structure of laminar counter-flow flames



Laminar counter-flow flames 1/3

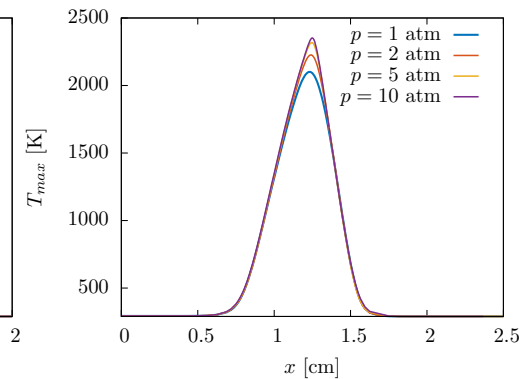
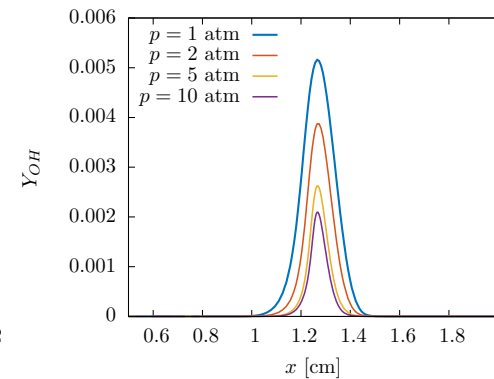
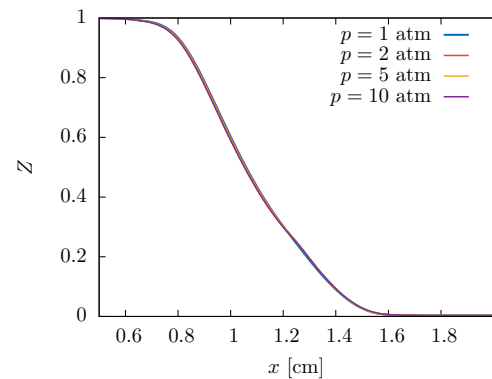
Counter-flow flames:

- **Oppdif** solver using a 12 species and 33 reactions (Li et al., 2007) and detailed transport
- Two series of flames simulated from 1 to 10 atm (1, 2, 5, 10 atm) consistently with experiments and LES campaigns



Series A: constant mass flow rate (Re)

Series B: constant inflow velocity ($U=25$ cm/s)



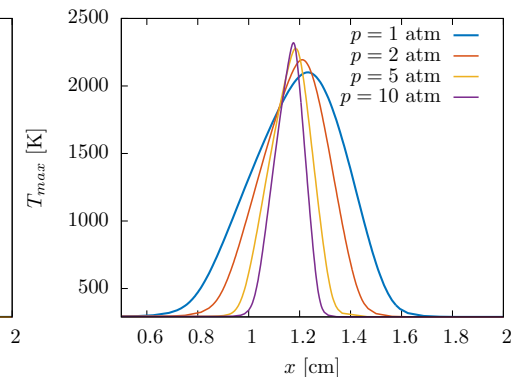
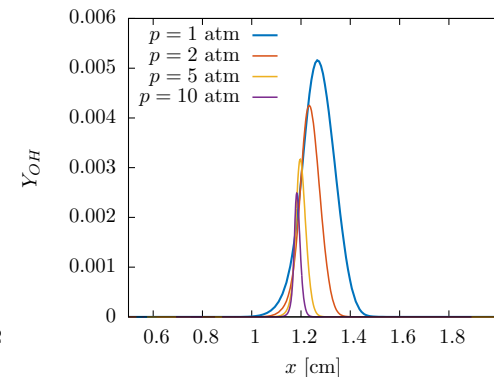
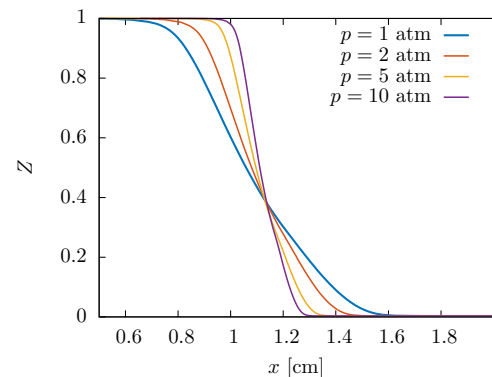
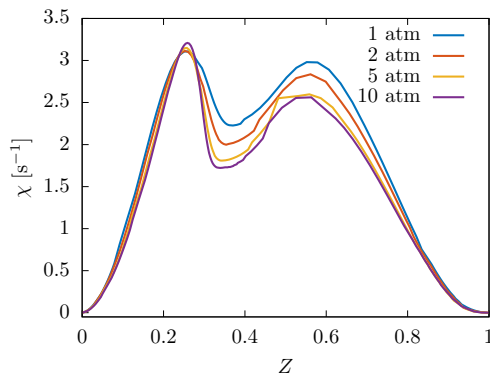
Molecular diffusivity decrease ($D \propto 1/\rho$)

- **A:** mixture fraction gradients const $\rightarrow$ **lower scalar dissipation**
- **B:** mixture fraction gradients increase $\rightarrow$ **constant scalar dissipation** (D and $\text{grad}(Z)$ compensate)

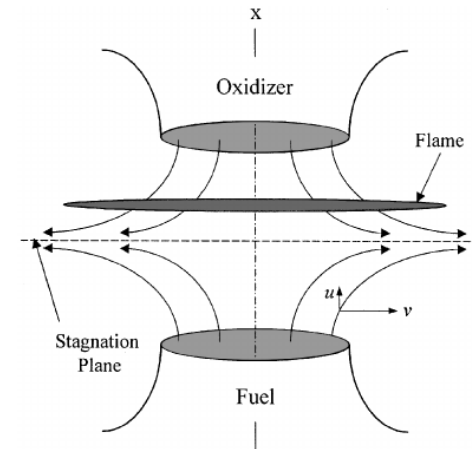
Flame thickness decrease
(higher mixture fraction gradients)

Temperature increase

Radical species decrease

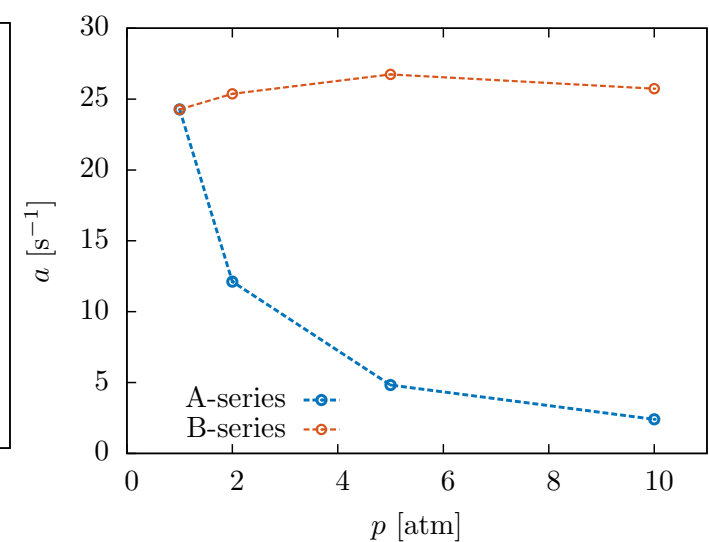
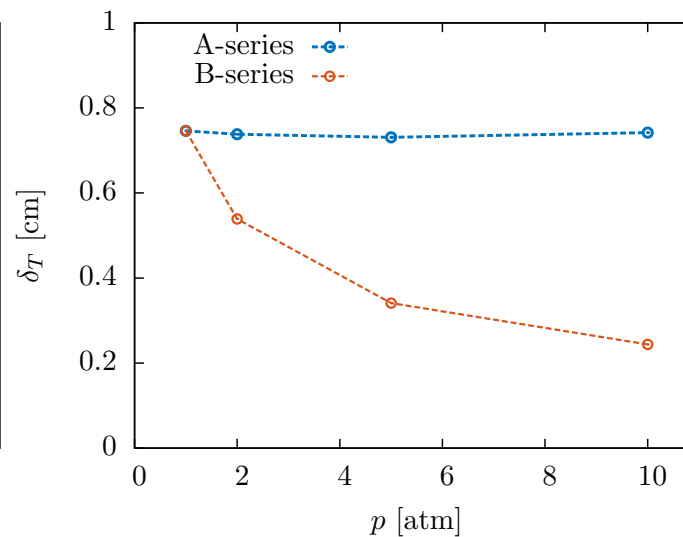
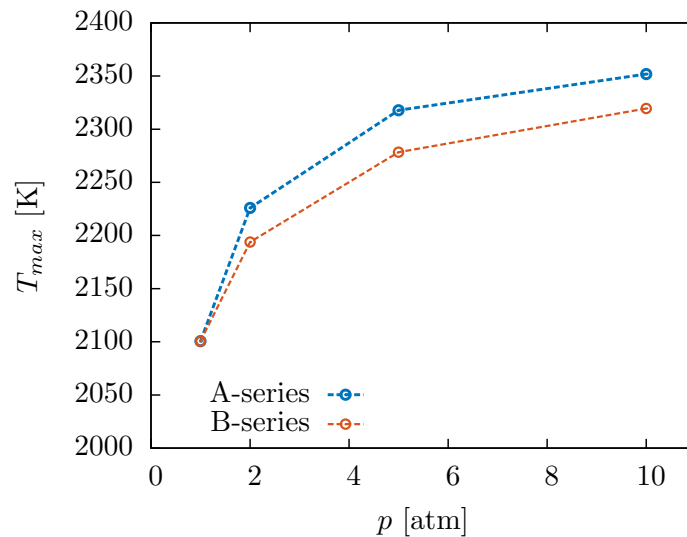


Laminar counter-flow flames 2/3



Counter-flow flames:

- **Oppdif** solver using a 12 species and 33 reactions (Li et al., 2007) and detailed transport
- Two series of flames simulated from 1 to 10 atm (1, 2, 5, 10 atm) consistently with experiments and LES campaigns

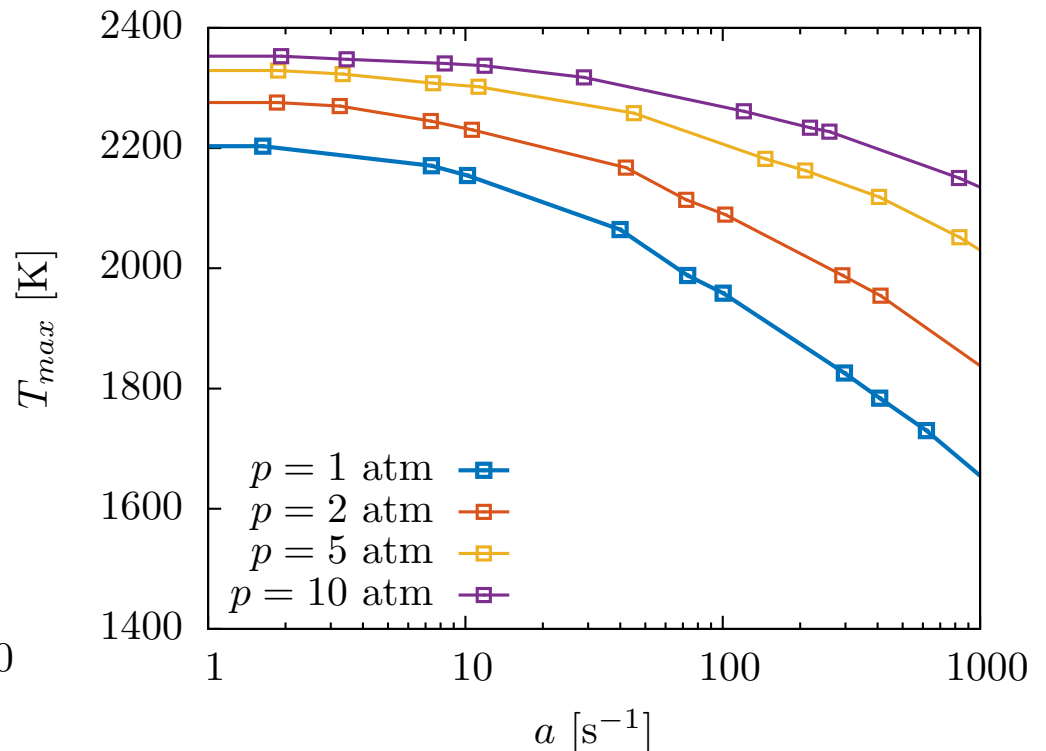
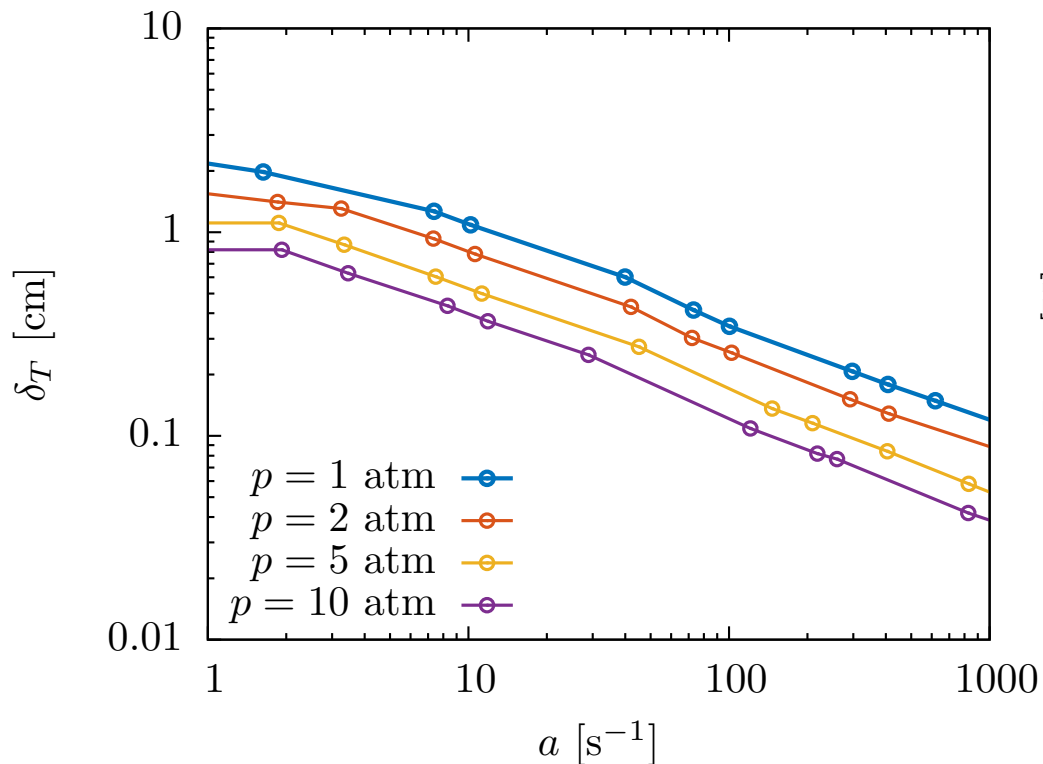


- Maximum **Temperature** increase similarly in both series
- **Flame thickness** essentially constant in series A (constant Flow rate) and decreases in series B (constant velocity)
- On the contrary **strain rate** decreases in series A (constant Flow rate) and essentially constant in series B (constant velocity)

Laminar counter-flow flames 3/3

Globally (if inflow velocity is varied) the pressure increase leads to:

- for a given pressure, thermal thickness decreases with strain rate a [s^{-1}]
- for a given strain rate, thermal thickness decreases with pressure
- high pressure counter-flow flame is more robust to strain (weaker dependence of T_{max} on a)



Sensitivity on pressure of chemical time-scales

CSP/TSR analysis on flamelet solutions 1/2



$$\frac{\partial Y_\alpha}{\partial t} = \frac{1}{2} \chi \frac{\partial^2 Y_\alpha}{\partial \xi^2} + \frac{\dot{\omega}_\alpha}{\rho}, \quad \alpha = 1, \dots, N_s$$

$$\frac{\partial T}{\partial t} = \frac{1}{2} \chi \left(\frac{\partial^2 T}{\partial \xi^2} + \frac{1}{c_p} \frac{\partial c_p}{\partial \xi} \frac{\partial T}{\partial \xi} \right) + \frac{\dot{\omega}_T}{c_p \rho}$$

- $\mathbf{x} = \{Y_\alpha, T\}$ state vector
- $\mathbf{g}(\mathbf{x})$ chemical source term
- $\mathbf{J}_g$ — of $\mathbf{g}(\mathbf{x})$
- $\mathbf{J}_g = \mathbf{A} \mathbf{\Lambda} \mathbf{B}$
- $\mathbf{A}, \mathbf{B}$ right and left eigenvector matrix of $\mathbf{J}_g$
- $\mathbf{\Lambda}$ eigenvalue matrix of $\mathbf{J}_g$
- $\mathbf{L}(\mathbf{x})$ diffusive term

Tangential Stretching Rate (TSR) extension to reaction-diffusion systems

- **Weighted average of the chemical source term Jacobian eigenvalues**
- **TSR:** reciprocal of the most energetic time scale associated with the **chemical source term**
- **Extended TSR** reciprocal of the most energetic time scale of the **reaction-diffusion system**

$$\frac{\partial \mathbf{x}}{\partial t} = \mathbf{L}(\mathbf{x}) + \mathbf{g}(\mathbf{x}), \quad \text{BCs on } \mathbf{x}, \quad \mathbf{x}(0) = \mathbf{x}_0$$

$$\frac{\partial \mathbf{x}}{\partial t} = \sum_{i=1, N} \mathbf{a}_i(\mathbf{x}) h^i(\mathbf{x}) \quad h^i = \mathbf{b}^i \cdot (\mathbf{L}(\mathbf{x}) + \mathbf{g}(\mathbf{x}))$$

$$\tilde{\tau}_{ext} =: \frac{\mathbf{L}(\mathbf{x}) + \mathbf{g}(\mathbf{x})}{|\mathbf{L}(\mathbf{x}) + \mathbf{g}(\mathbf{x})|}$$

$$W_{i,ext} =: \frac{h^i}{L + g} (\tilde{\tau}_{ext} \cdot \mathbf{a}_i) = \frac{h^i}{L + g} \sum_{k=1}^N \frac{h^k}{L + g} (\mathbf{a}_k \cdot \mathbf{a}_i)$$

$$\omega_{\tilde{\tau}_{ext}} := \tilde{\tau}_{ext} \cdot \mathbf{J}_g \cdot \tilde{\tau}_{ext} = \sum_{i=1}^N W_{i,ext} \lambda_i$$

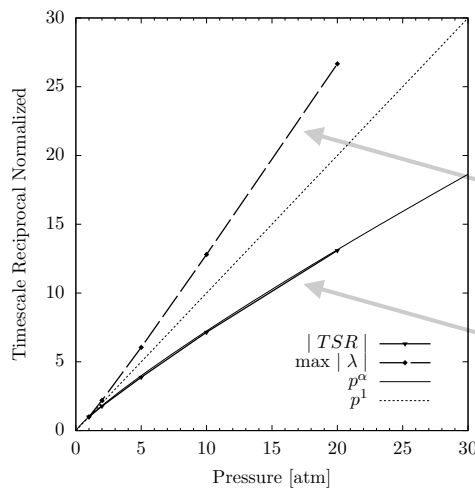
Sensitivity of chemical time-scales to pressure

CSP/TSR analysis on flamelet solutions 2/2



Pressure increase leads to:

- higher temperatures and **smaller timescales**
- **shrinking of the region** where the system dynamics is **governed by chemical kinetics** (where the TSR and the extended TSR coincide)
- closer to infinitely fast limit

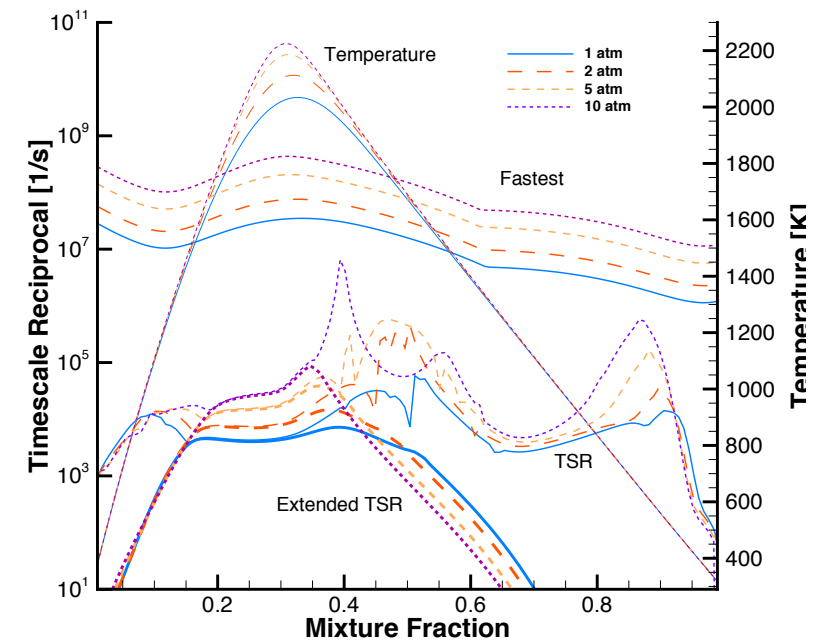


At stoichiometric mixture fraction ($Z_{st}=0.295$):

- reciprocal of fastest time scale follows a power law with exponent larger than one
- **TSR (most energetic chemical timescale), follows a power law with exponent $\alpha=0.86$**

Test cases:

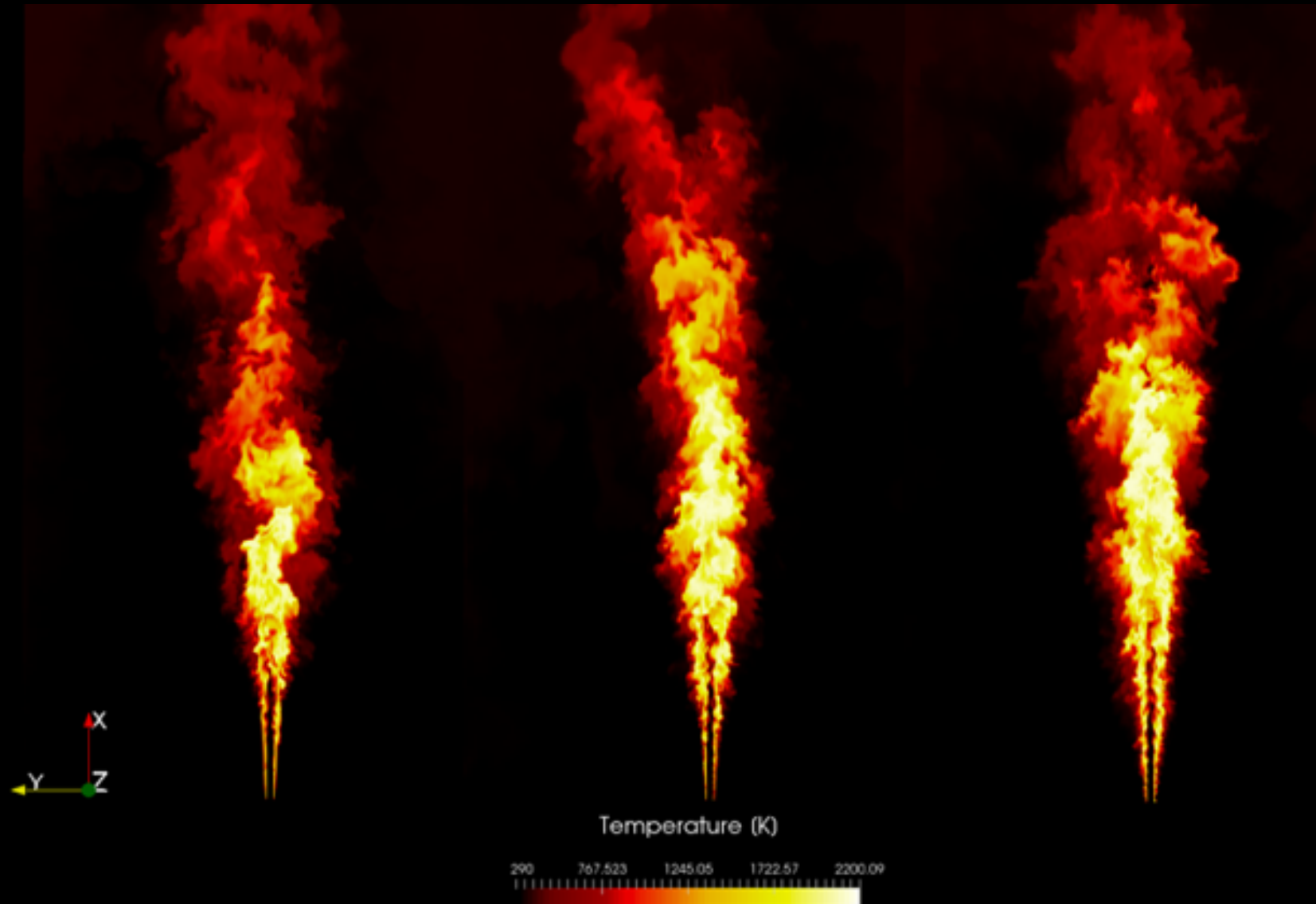
- **SDR = 10s^{-1}**
- **P = 1, 2, 5, 10 atm**



- decrease in scalar dissipation and increase in TSR

➔ Damkhöler number increase (**Steady laminar flamelet approach justified for higher p**)

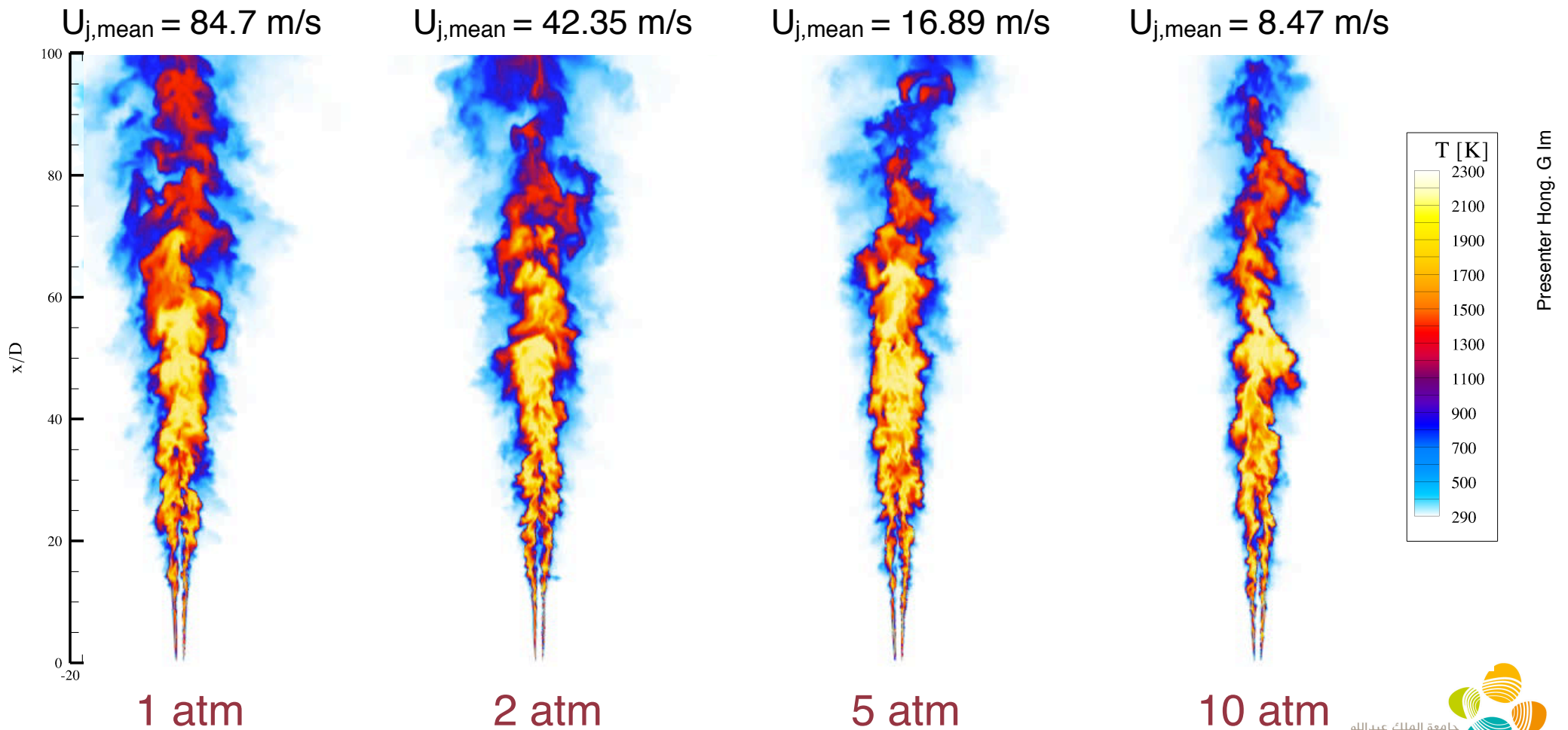
Series A: increasing pressure - constant Reynolds number ($p = 2, 5, 10$ atm)



Series A: increasing pressure - constant Re (1/7)

Pressure increase leads to:

- higher density with constant dynamic viscosity μ
- **Re** kept constant, decreasing velocity to compensate the density increase (constant flow rate)



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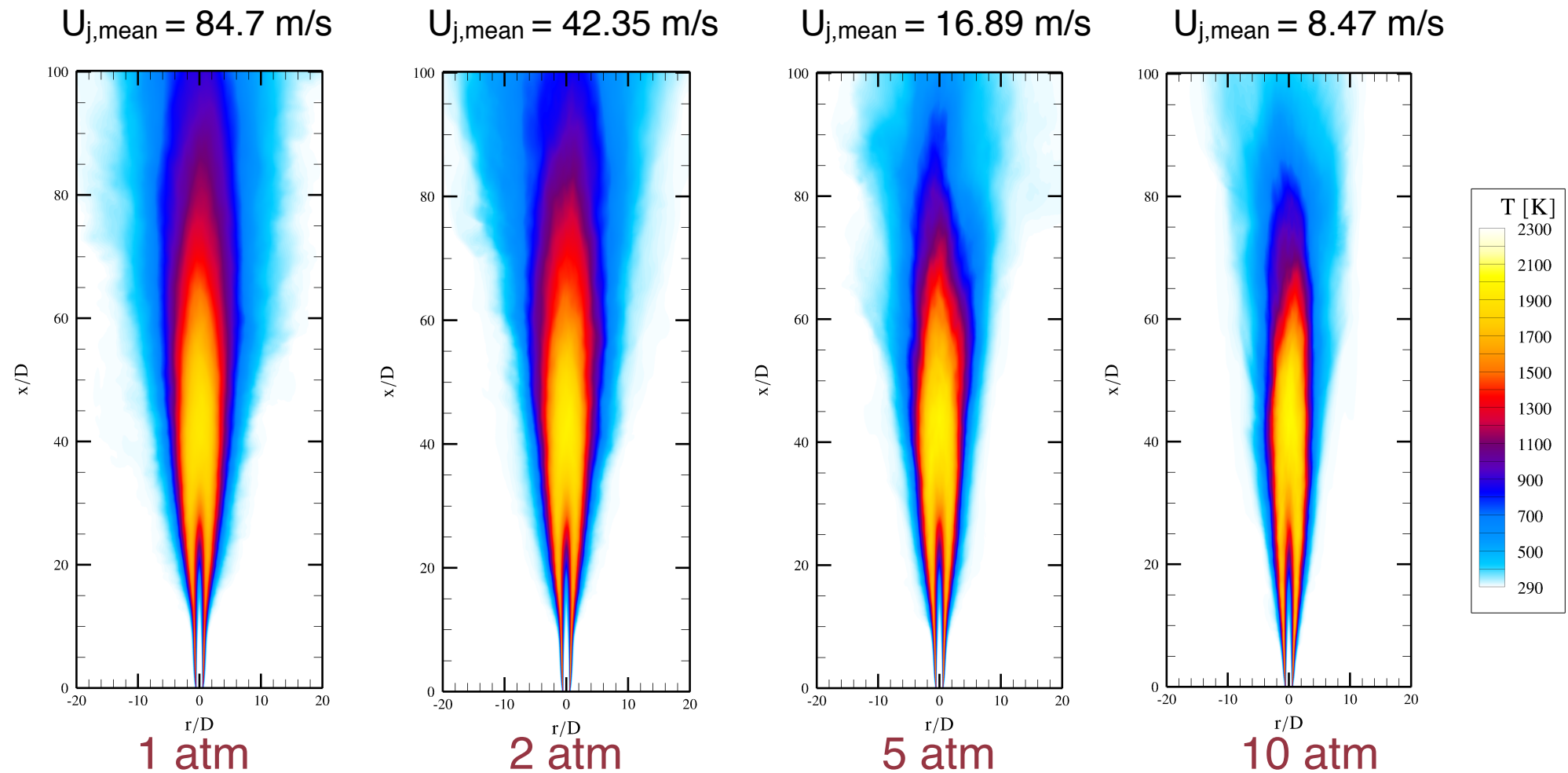


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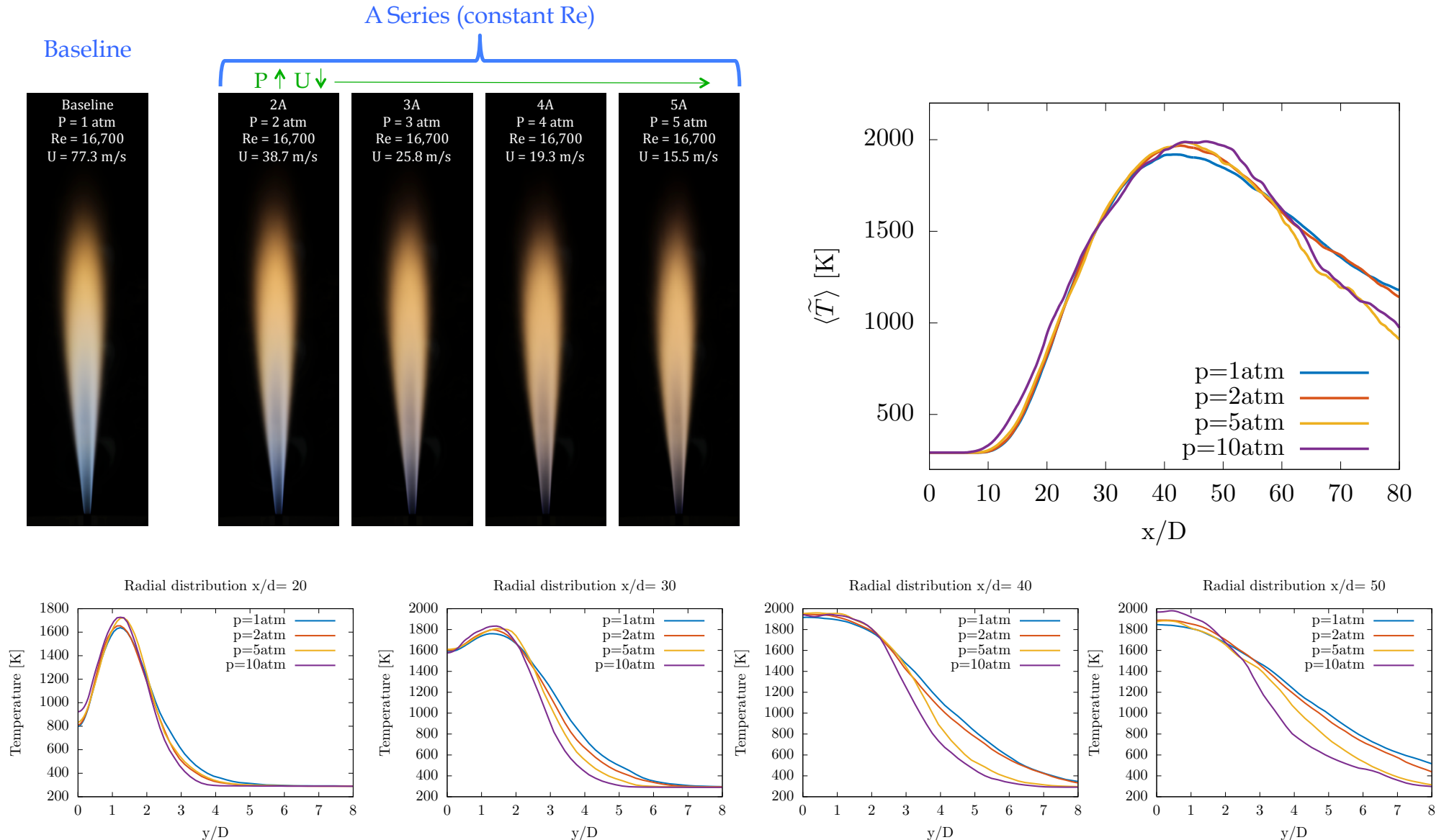
Series A: increasing pressure - constant Re (2/7)

- The pressure increase leads to shorter flames
- The same amount of fuel mass is burned in a more confined spatial region



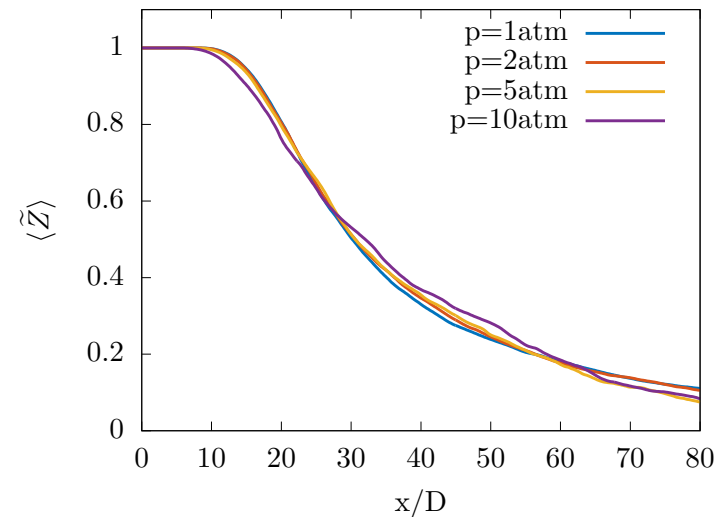
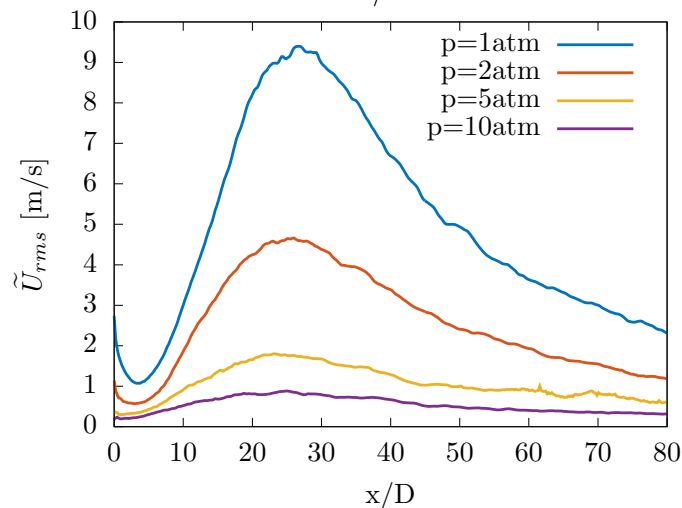
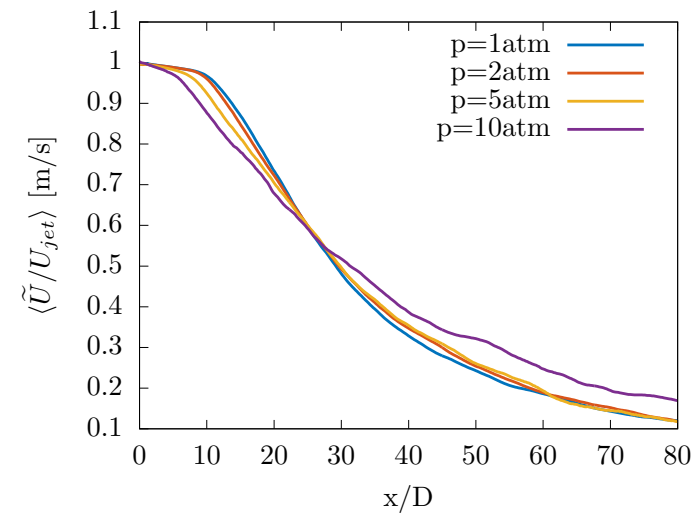
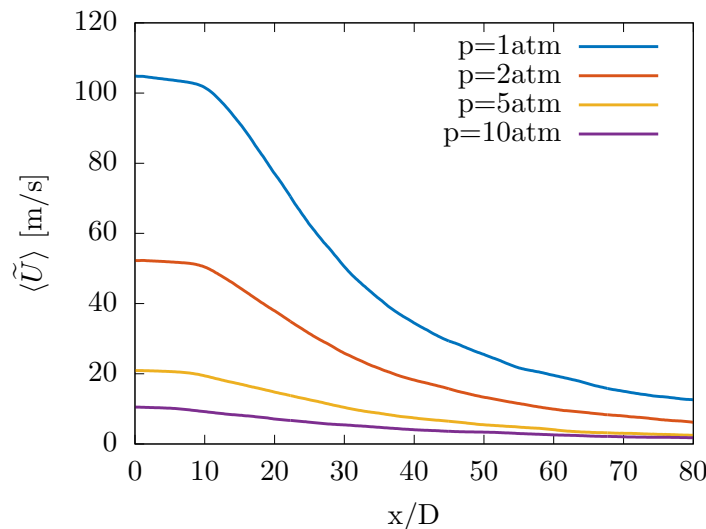
Series A: increasing pressure - constant Re (3/7)

- Averages of predicted temperature seem to correctly reproduce the preliminary experimental results



Series A: increasing pressure - constant Re (4/7)

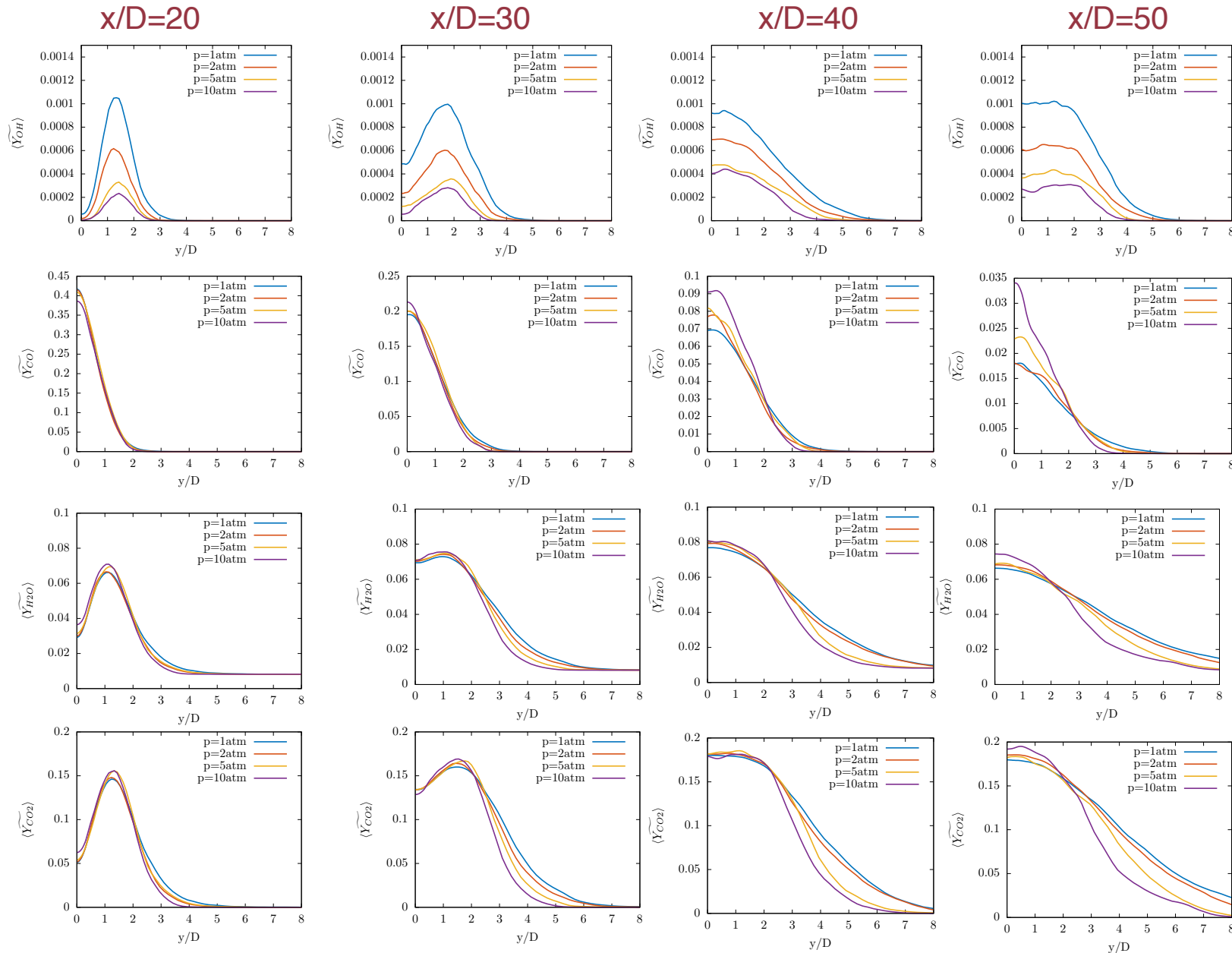
- Axial distribution of mean velocity and of its standard deviation display a qualitatively similar decrease with pressure
- Earlier velocity decrease at $x/D \approx 10$
- Axial distribution of mean mixture fraction bearing close similarity



Series A: increasing pressure - constant Re (5/7)

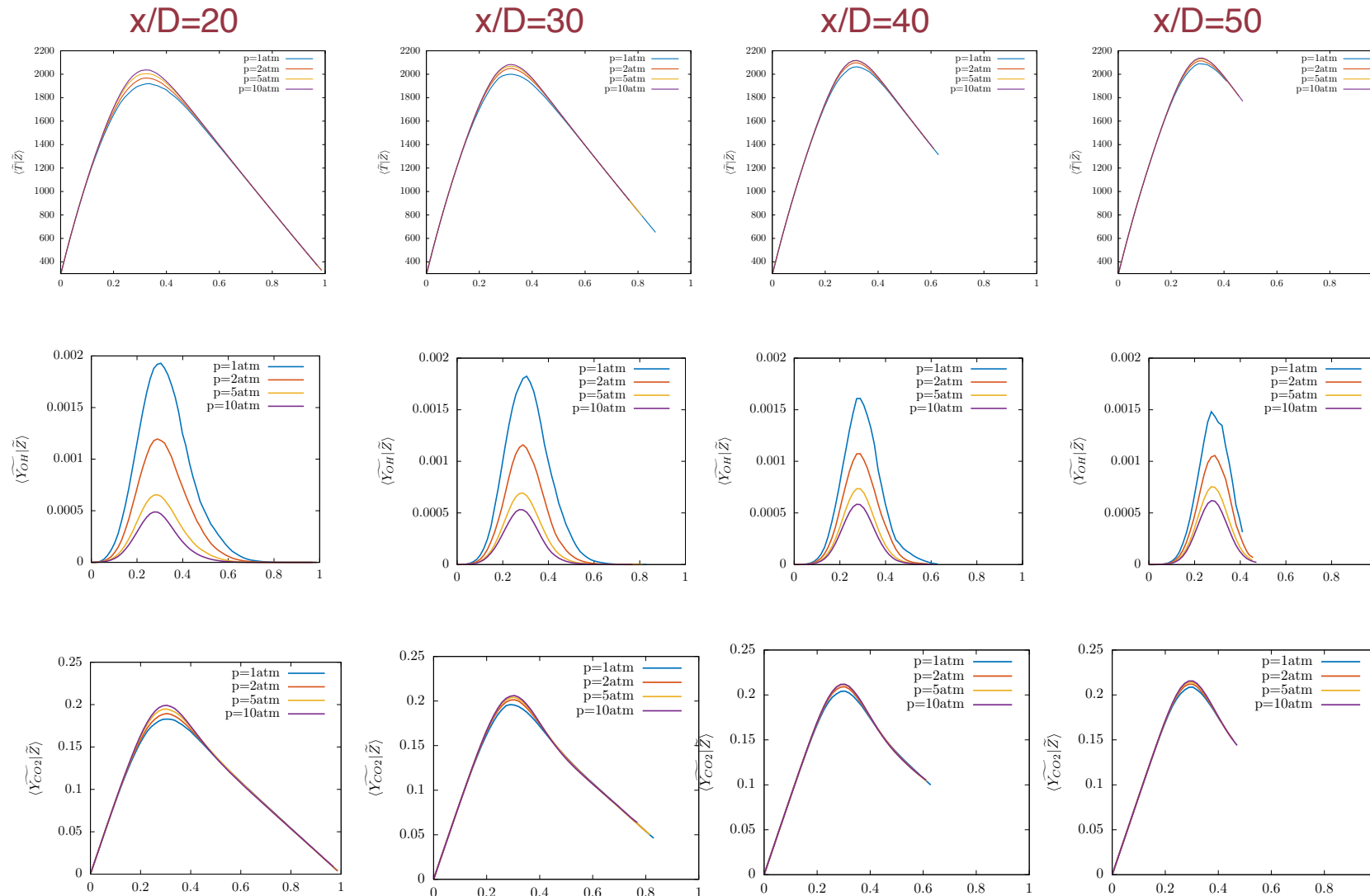


- Flame length clearly influences the species radial profiles



Series A: increasing pressure - constant Re (6/7)

- Species conditional averages highlight pressure influence on laminar chemistry (higher T and lower radicals concentration)



Temperature

increase in the region
close to the nozzle

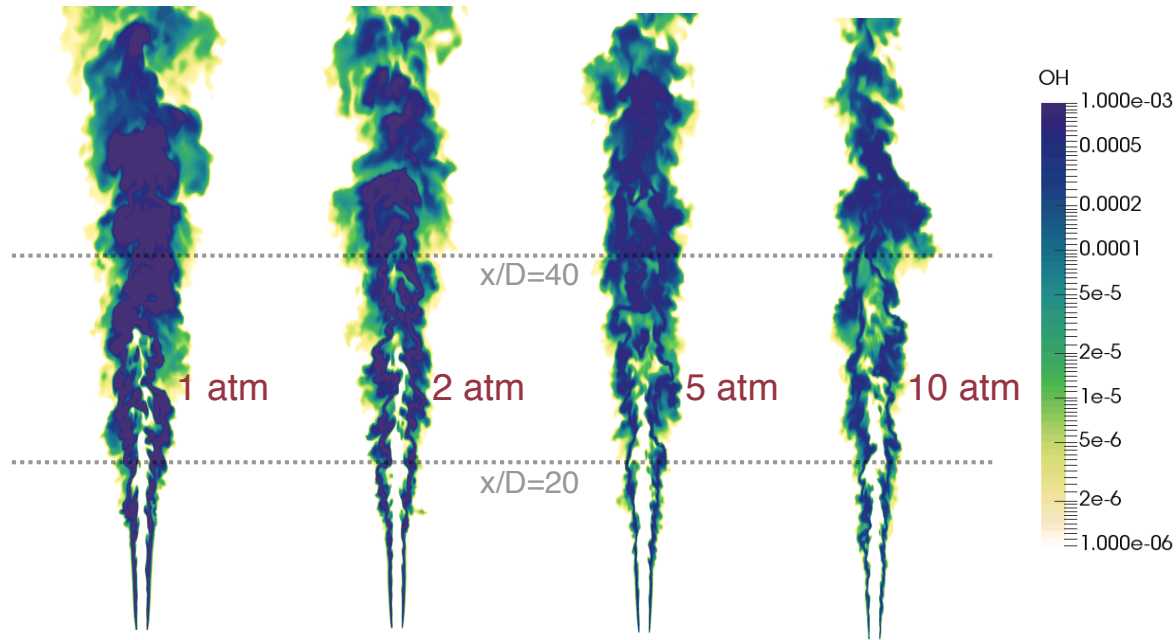
OH

decrease with pressure
consistent with what is
observed for the laminar
counterflow flames

CO₂

increase in the region
close to the nozzle

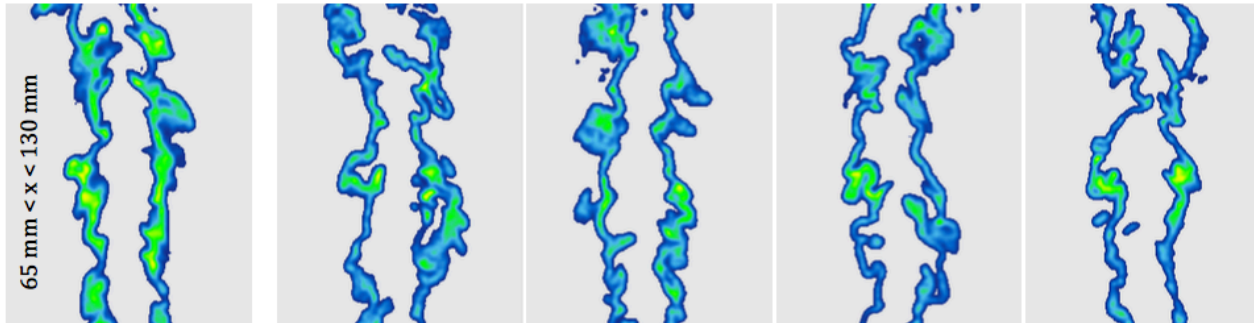
Series A: increasing pressure - constant Re (7/7)



Consistently with experimental results:

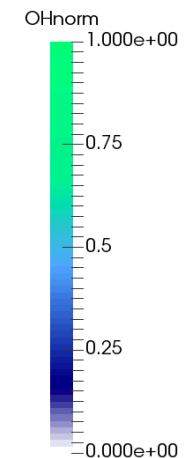
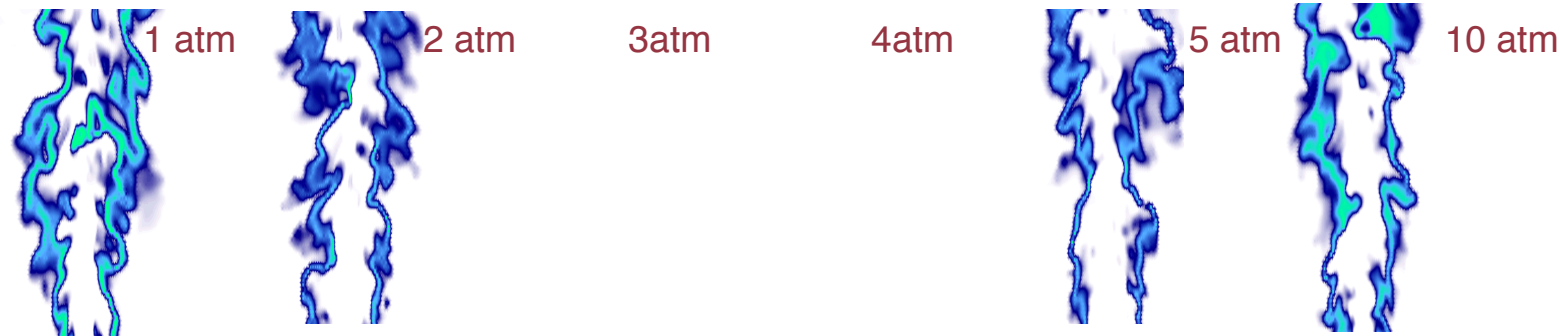
- Increasing wrinkling of OH layer as P increases
- Decreasing thickness of OH layer as P increases

experimental



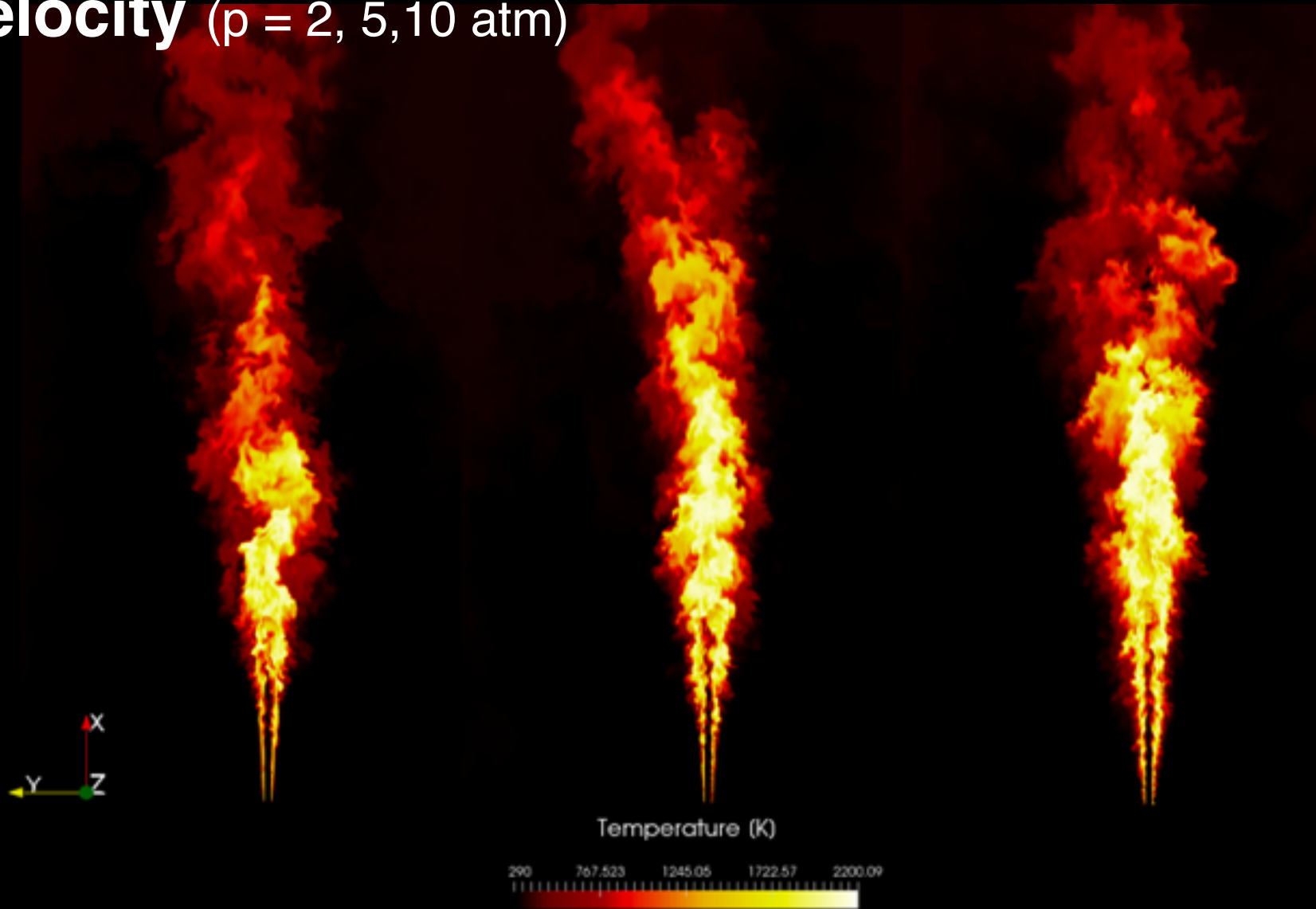
Qualitative agreement also
for normalized OH contours

LES



Series B: increasing pressure - constant velocity

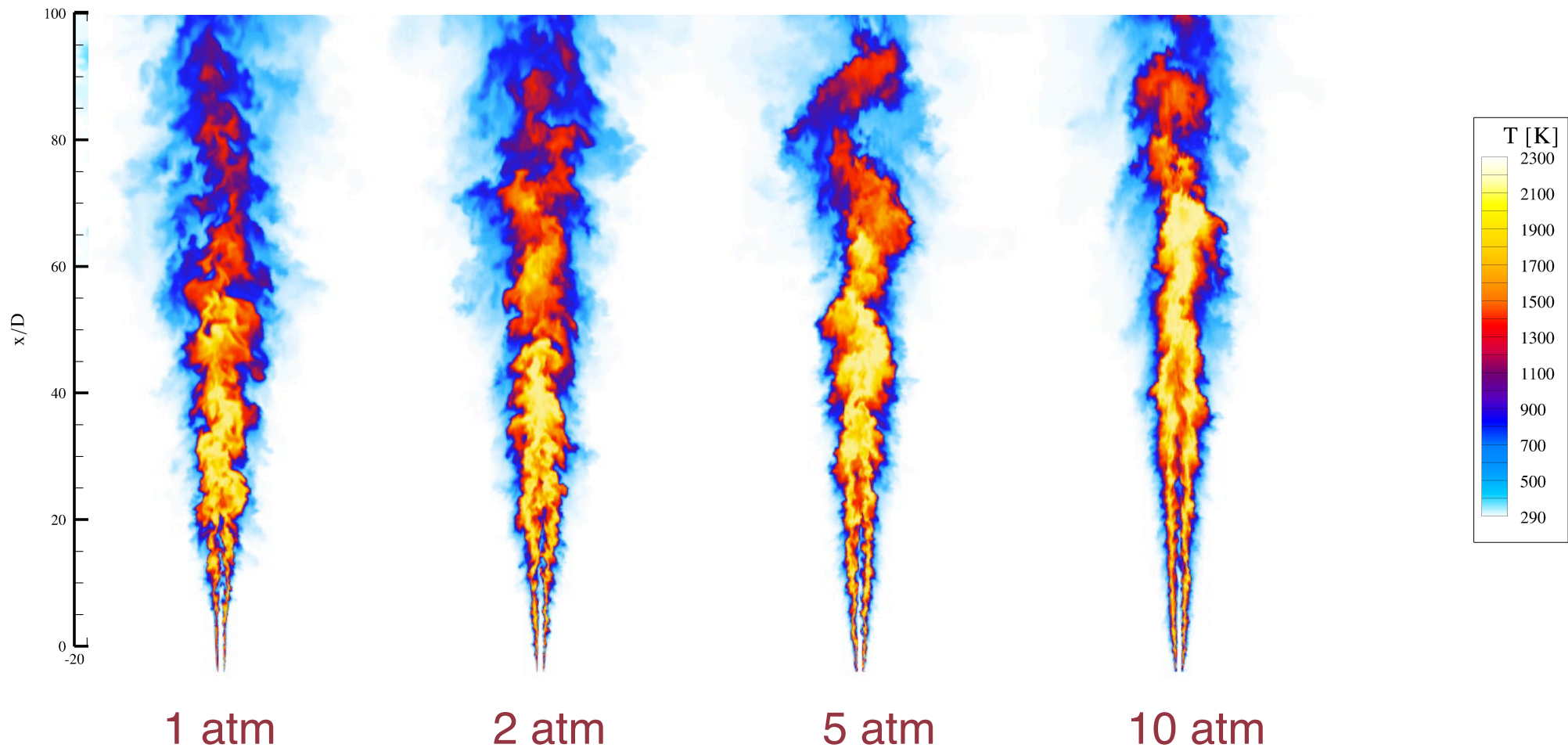
($p = 2, 5, 10$ atm)



Series B: increasing pressure - constant velocity (1/7)

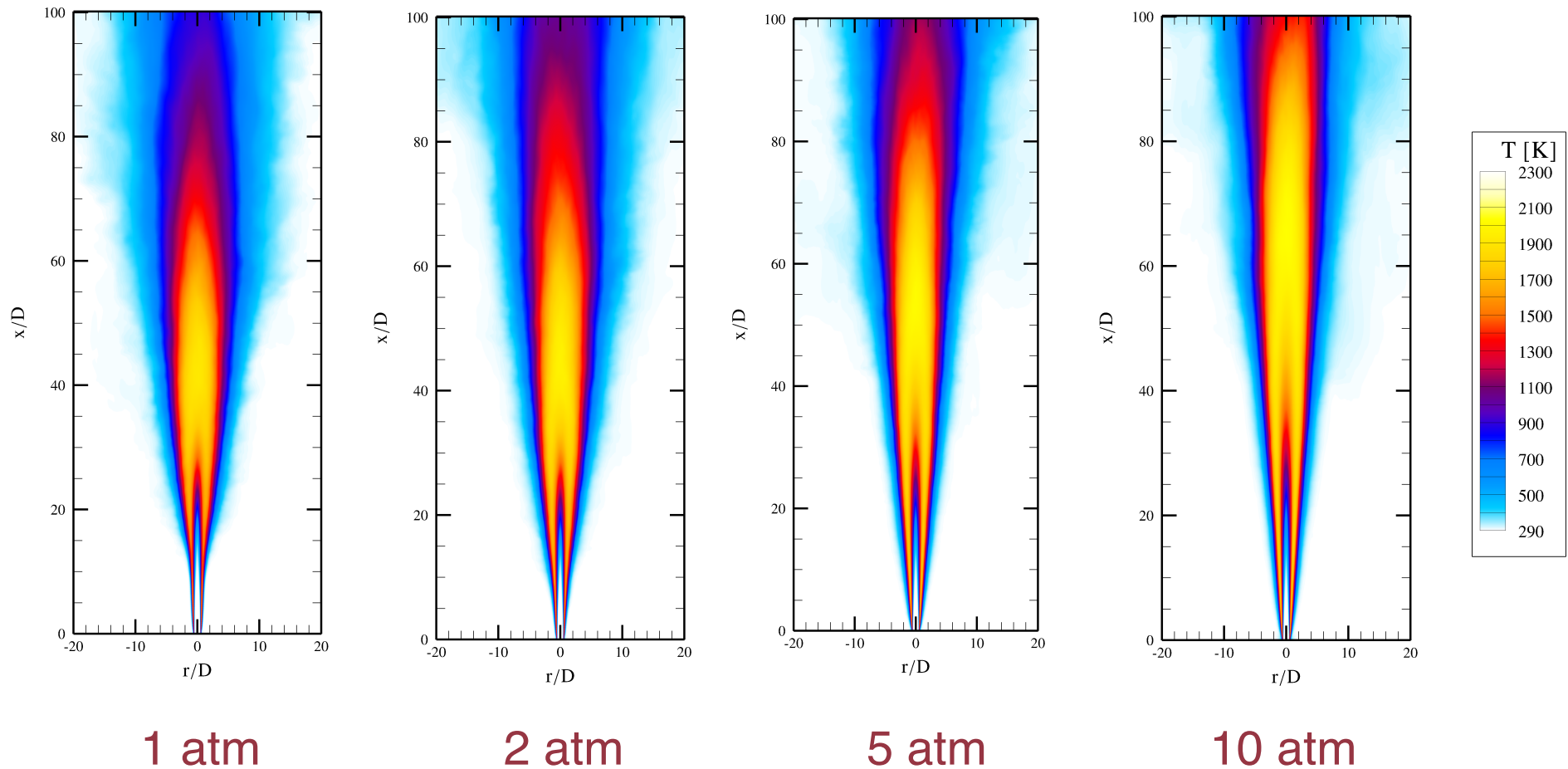
Pressure increase leads to:

- increase in Reynolds number and, as a consequence, the mass flow rate
- finer structures are observed in high pressure simulations



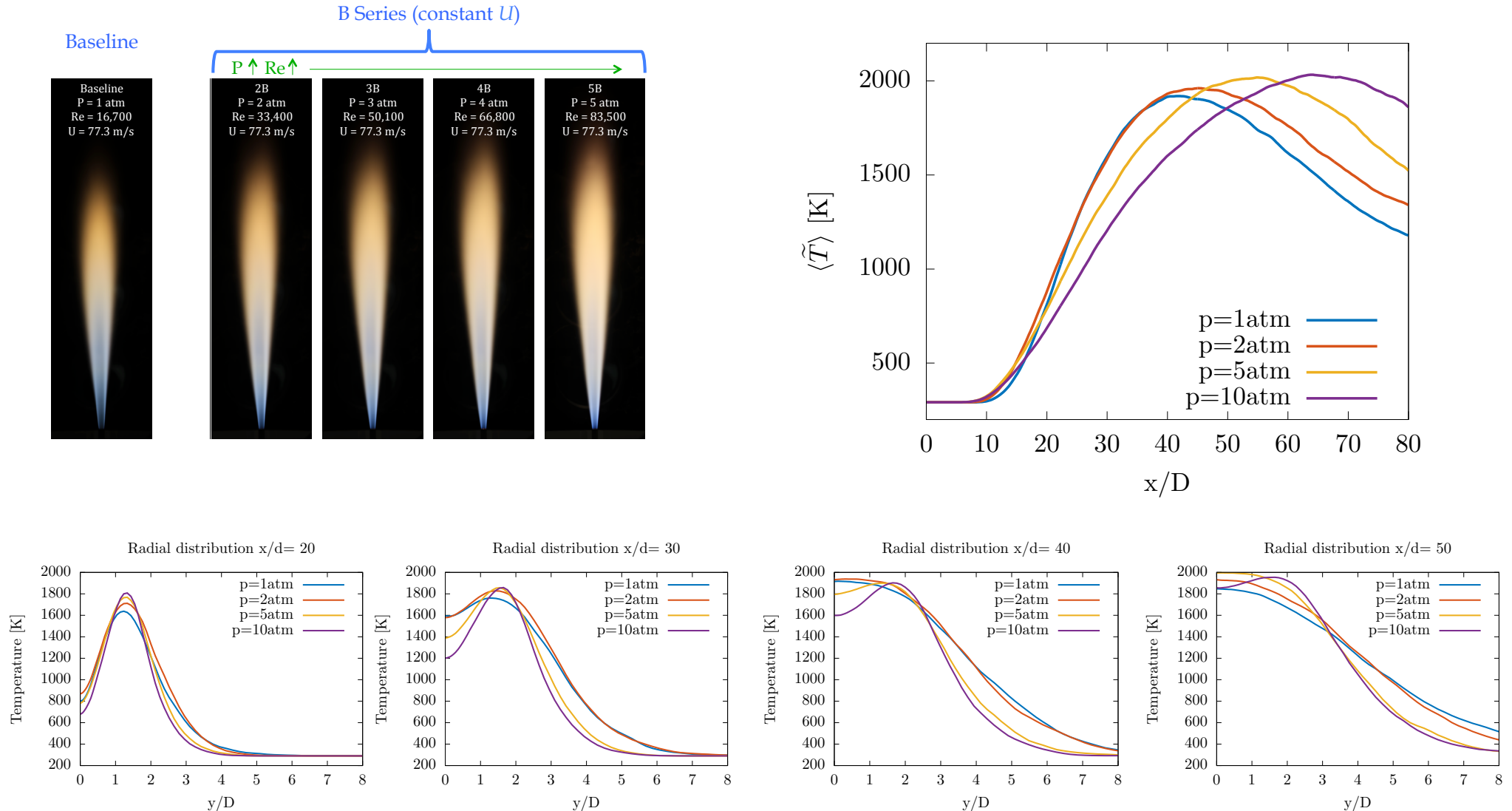
Series B: increasing pressure - constant velocity (2/7)

- The pressure increase leads to longer flames
- The spread angle of the reacting jet seems to be reduced

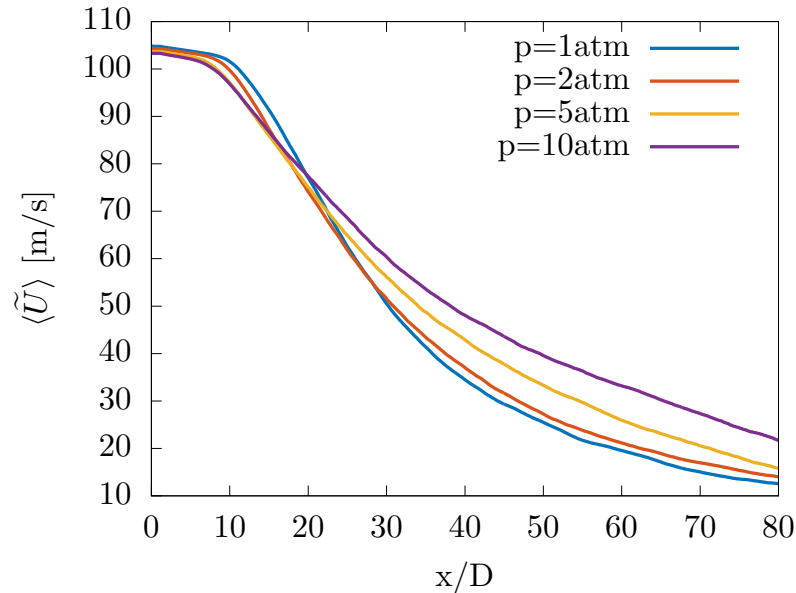


Series B: increasing pressure - constant velocity (3/7)

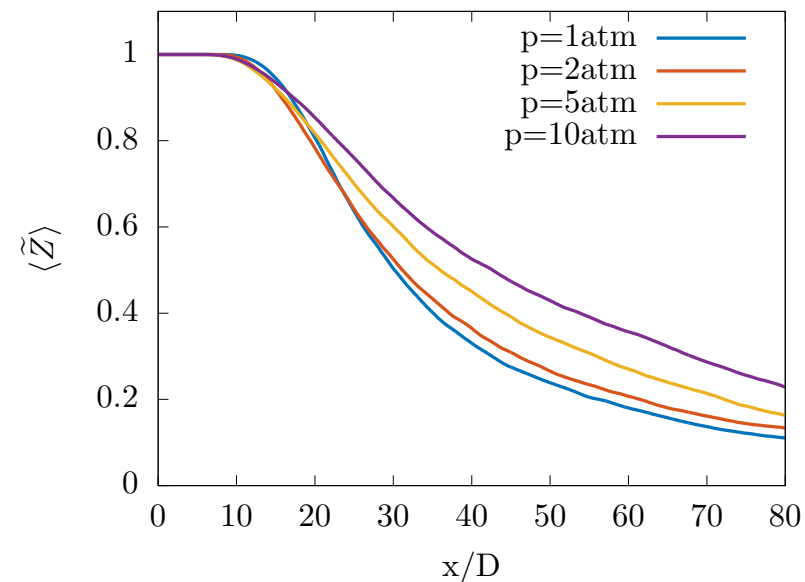
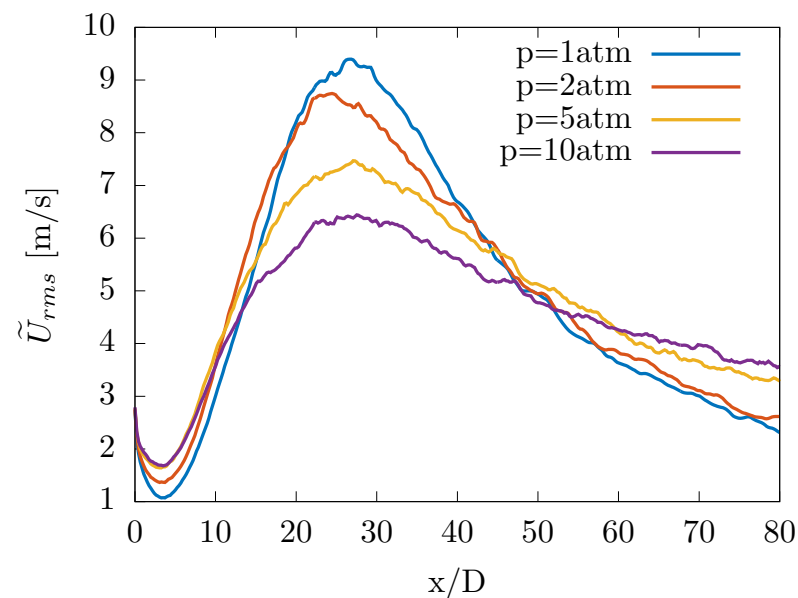
- Temperature peak occurs further downstream for higher pressures, showing consistency with preliminary experimental results



Series B: increasing pressure - constant velocity (4/7)



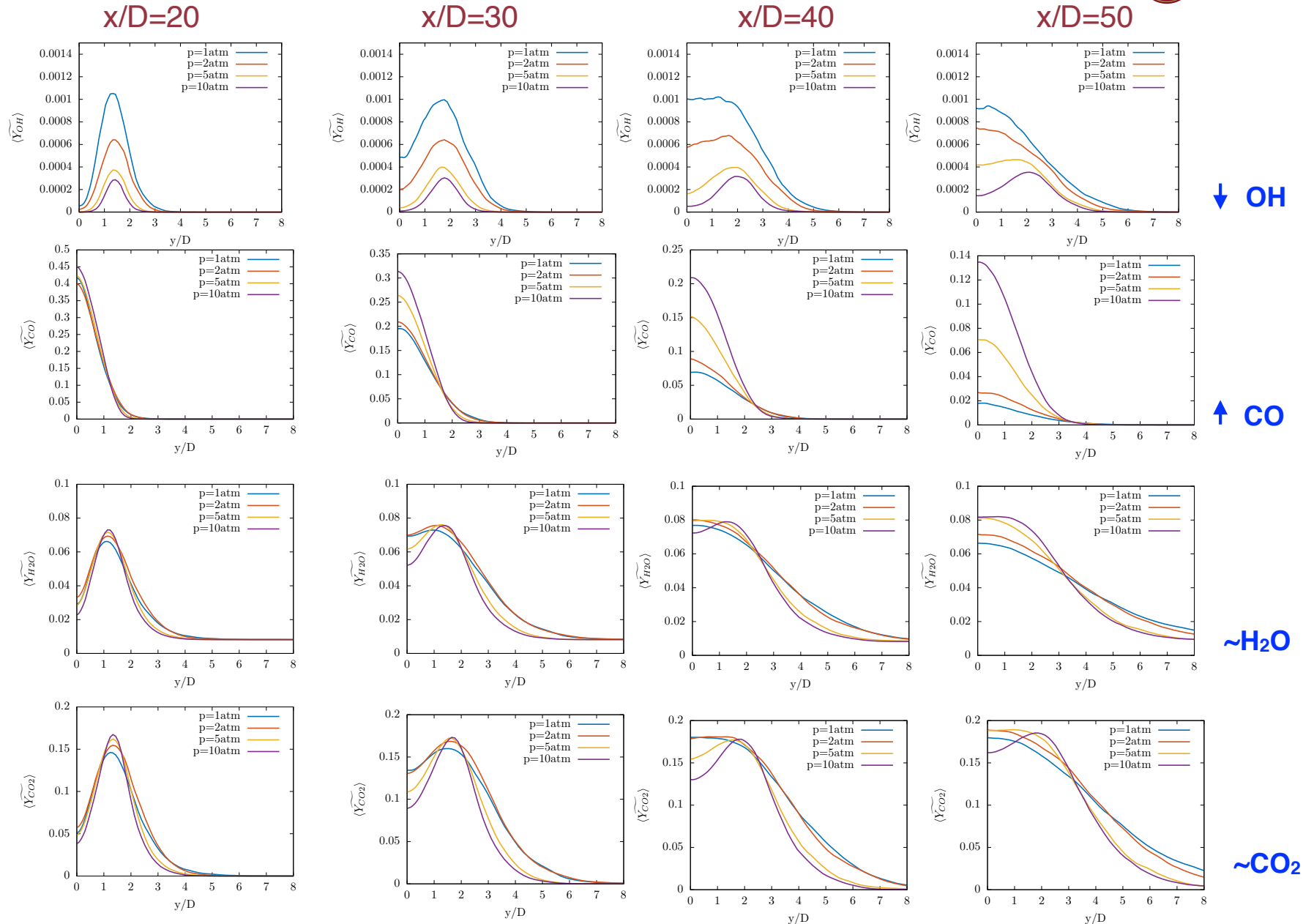
- Axial distribution of both mean and velocity fluctuations get flattened with pressure
- As a result, the drop in the mean mixture fraction along the axial direction is reduced as pressure increased (longer flames)



Series B: increasing pressure - constant velocity (5/7)

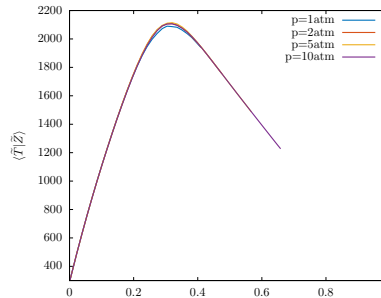
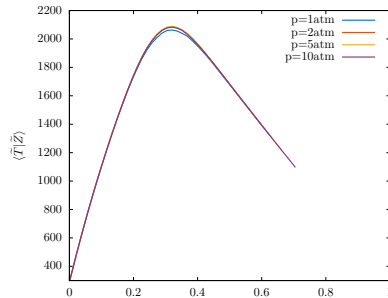
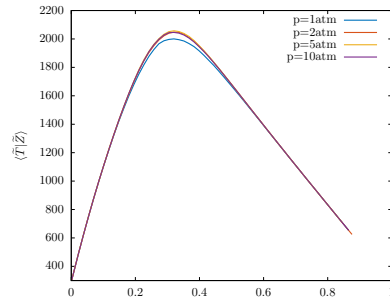
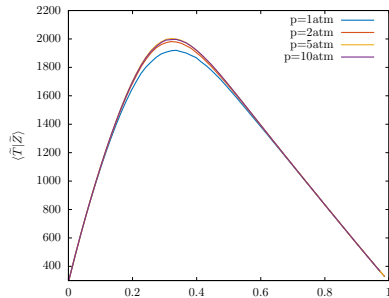


- Flame length clearly influences the species radial profiles



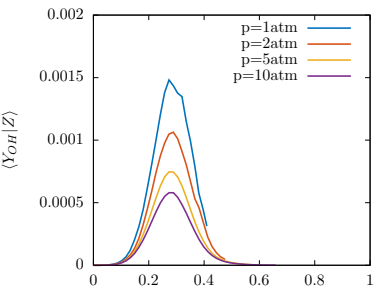
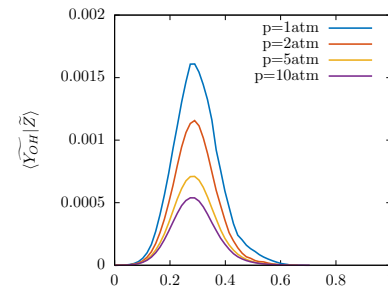
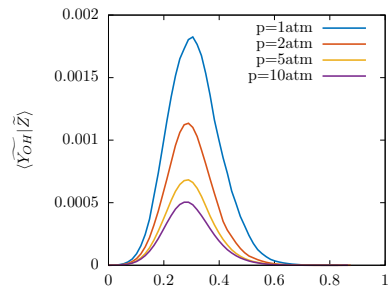
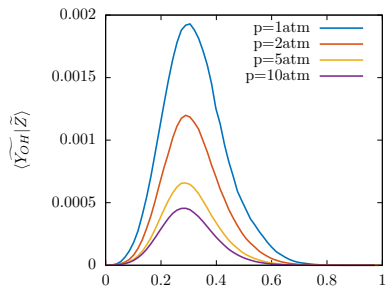
Series B: increasing pressure - constant velocity (6/7)

- Species conditional averages highlight pressure influence on laminar chemistry (higher T and lower radicals concentration)



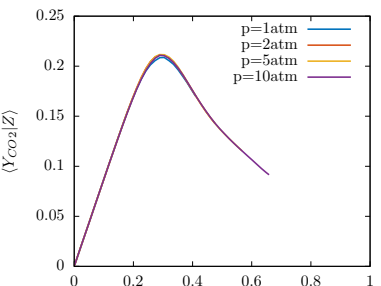
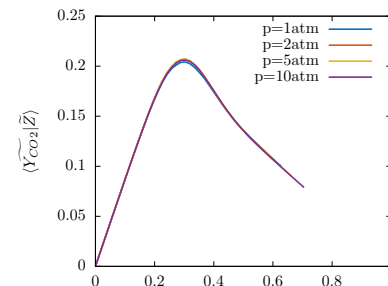
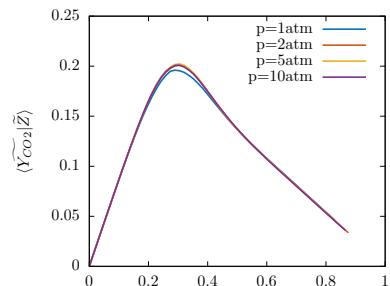
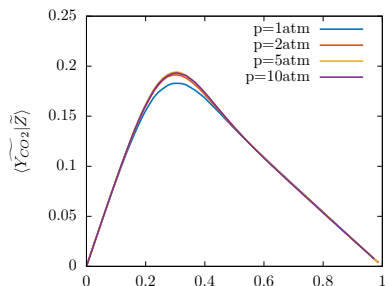
Temperature

minor increase in the
region close to the nozzle



OH

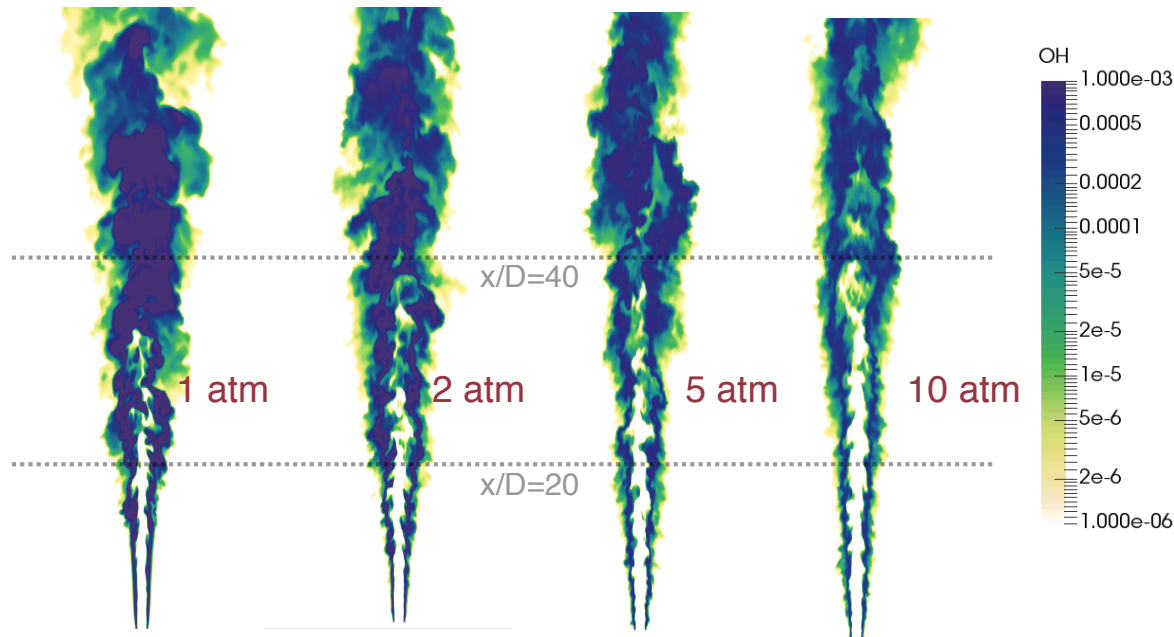
decrease with pressure
consistent with what is
observed for the laminar
counterflow flames



CO₂

minor increase in the
region close to the nozzle

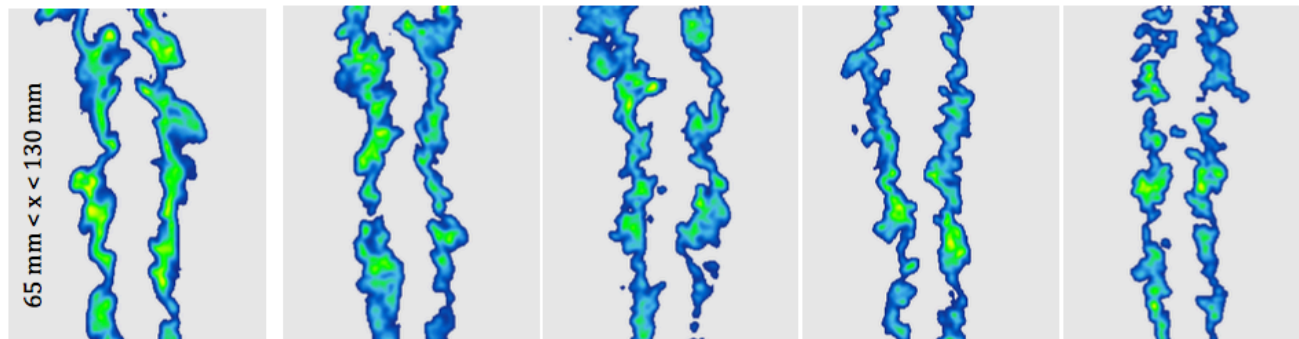
Series B: increasing pressure - constant Velocity (7/7)



Consistently with experimental results:

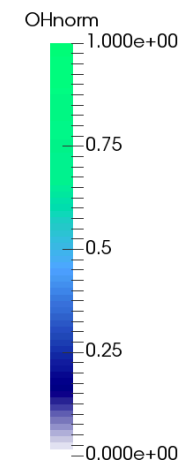
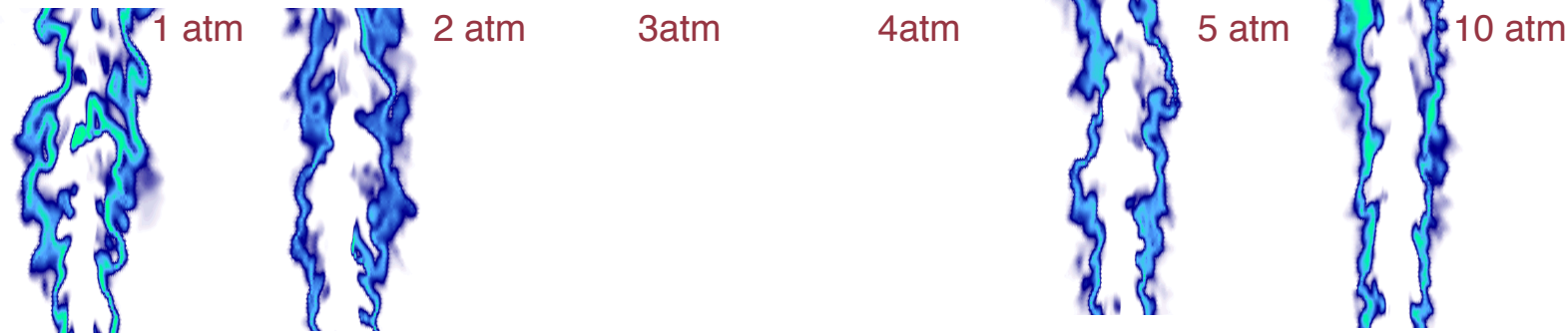
- Increasing wrinkling of OH layer as P & Re increases
- Decreasing thickness of OH layer as P & Re increases

experimental



**Qualitative agreement also
for normalized OH contours**

LES



Summary and conclusions

- High-pressure syngas/air flames were simulated using LES and a steady laminar flamelet model
- LES framework was validated against measurements of Sandia flame A at 1 atm
- Flamelet assumption for high-pressure syngas/air flames was assessed using the TSR concept - sub-linear increase in the energetic time scale
- Two simulation sets aligned with the on-going experimental effort in the Clean Combustion Research Center (CCRC) at KAUST:
 - ▶ **Series A** (constant Re) has shown shorter and generally more compact flames with increasing pressure
 - ▶ **Series B** (constant U) has shown longer and more strained flames with increasing pressure
 - ▶ For both series A & B, as pressure increases, peak temperature increases while OH, H₂O₂, and HCO decrease
- **LES outcomes are qualitatively consistent with preliminary experimental results**

What's next?

- Comparison of LES results with the on-going high-pressure CCRC experiments
- Consistent analysis of the jet break-up and spread angle as function of pressure
- Detailed simulation of high-pressure inlet and near field to investigate flame anchoring and pressure effect on hydrogen leakage

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