

# Numerical characterization of premixed methane flames in vitiated atmosphere at supercritical conditions

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## 3rd International Seminar on Non-Ideal Compressible-Fluid Dynamics for Propulsion & Power

Delft, 29th - 30th October 2020

### **Numerical characterization of premixed methane flames in vitiated atmosphere at supercritical conditions**

F. Lo Presti<sup>1</sup>, P. Post<sup>1</sup>, F. di Mare<sup>1</sup>, J. van Oijen<sup>2</sup>

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<sup>2</sup> *Department of Mechanical Engineering, Eindhoven University of Technology*

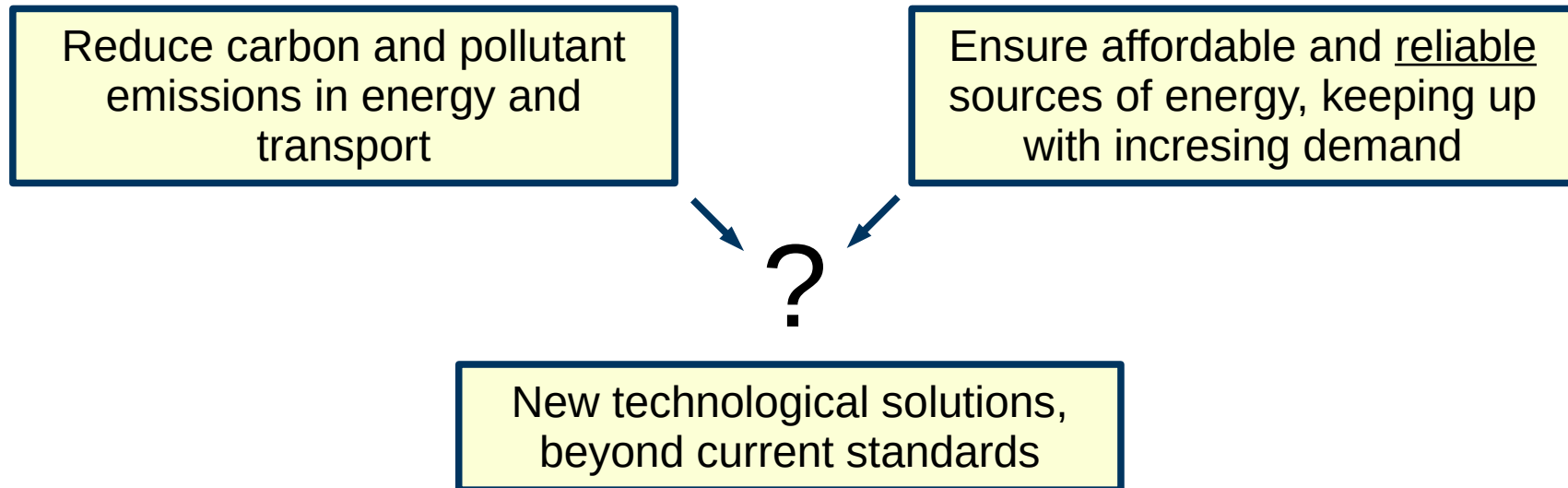


**RUHR-UNIVERSITÄT BOCHUM**

**CHAIR OF THERMAL TURBOMACHINES AND AEROENGINES**

# Introduction and motivation

Fundamental technological challenges in the next future

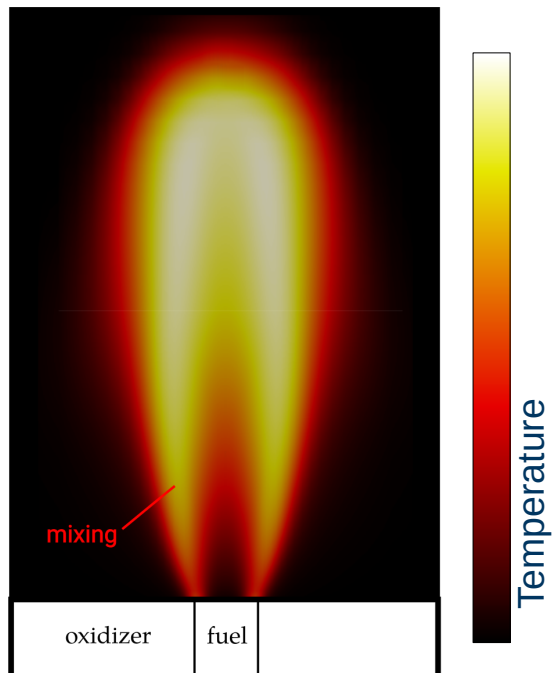


Some research trends in gas turbines:

- Hydrogen combustion
- Carbon Capture and Sequestration  
e. g. in directly fired supercritical CO<sub>2</sub> power cycles {
  - reduce CO<sub>2</sub> emissions
  - oxyfuel: no NO<sub>x</sub>
  - higher density: lower size

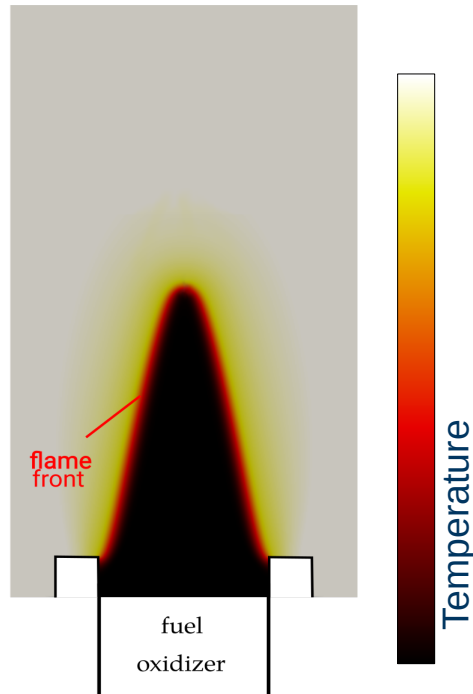
# Introduction and motivation

## Non-premixed



Most application of supercritical combustion

## Premixed



Unexplored field at very high pressures

Stability critical issue

## **Purpose:**

Characterize flame properties

Develop numerical model for stability studies

# Outline

- Introduction and Motivation
- One dimensional flames:
  - Chemistry solver
  - Chemistry mechanisms
  - Equation of state, thermodynamics and transport
- Two dimensional application
  - Coupling CFD and chemistry solver
  - Bunsen flames results
- Conclusions and outlook

# Outline

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# One dimensional flames

## Chemistry solver

### CHEM1D<sup>1</sup>

- One-dimensional laminar flame code
- Complex chemistry reaction mechanisms

### Extended with

- Peng Robinson EOS with consistent thermodynamics
- High pressure Chung's method for mixture transport properties

<sup>1</sup>CHEM1D, A one-dimensional laminar flame code, Eindhoven University of Technology. <http://www.combustion.tue.nl/chem1d>

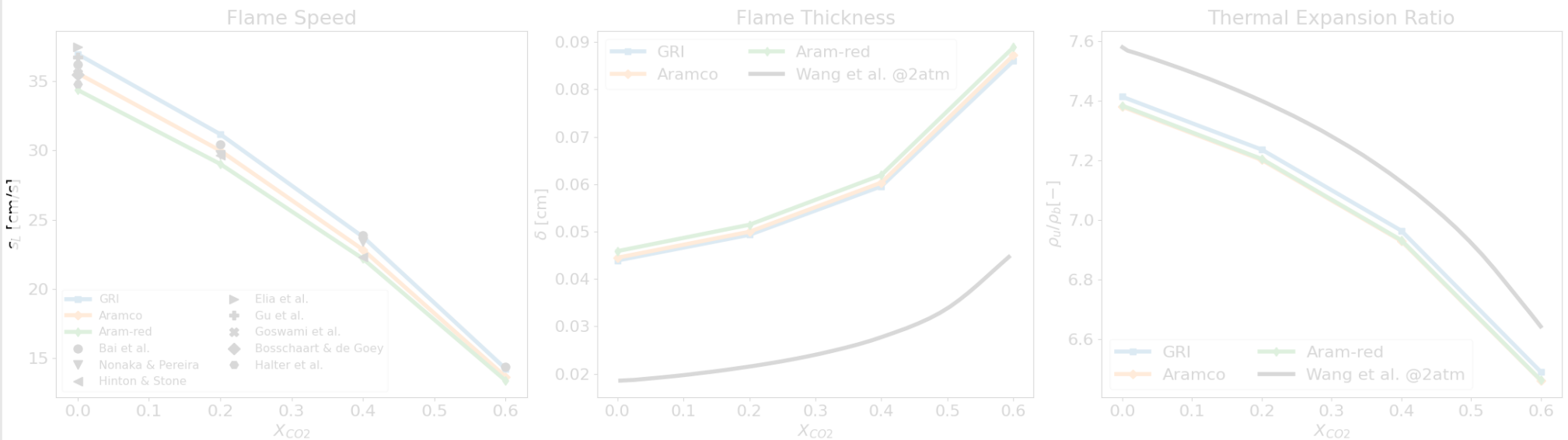
# One dimensional flames

## Biogas mixtures

$\Phi$	Fuel		Oxidizer		
	CH <sub>4</sub>	CO <sub>2</sub>	N <sub>2</sub>	O <sub>2</sub>	Ar
1.0	1.0	0.0	0.781	0.21	0.009
1.0	0.8	0.2	0.781	0.21	0.009
1.0	0.6	0.4	0.781	0.21	0.009
1.0	0.4	0.6	0.781	0.21	0.009

Unburnt mixture T=300K

### Validation at low pressure





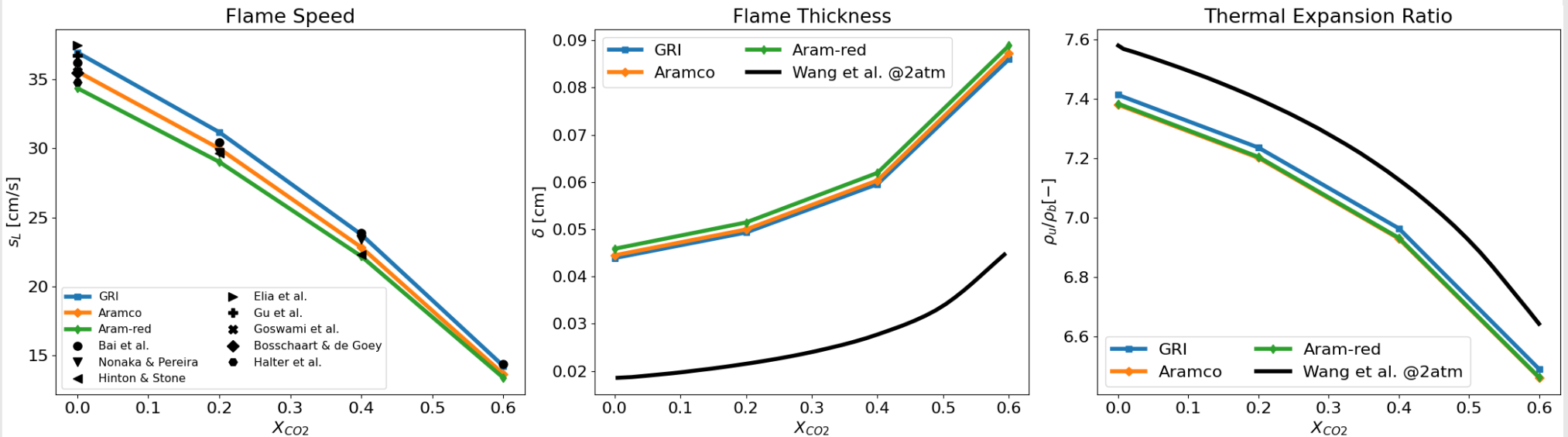
# One dimensional flames

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1.0	0.4	0.6	0.781	0.21	0.009

Unburnt mixture T=300K

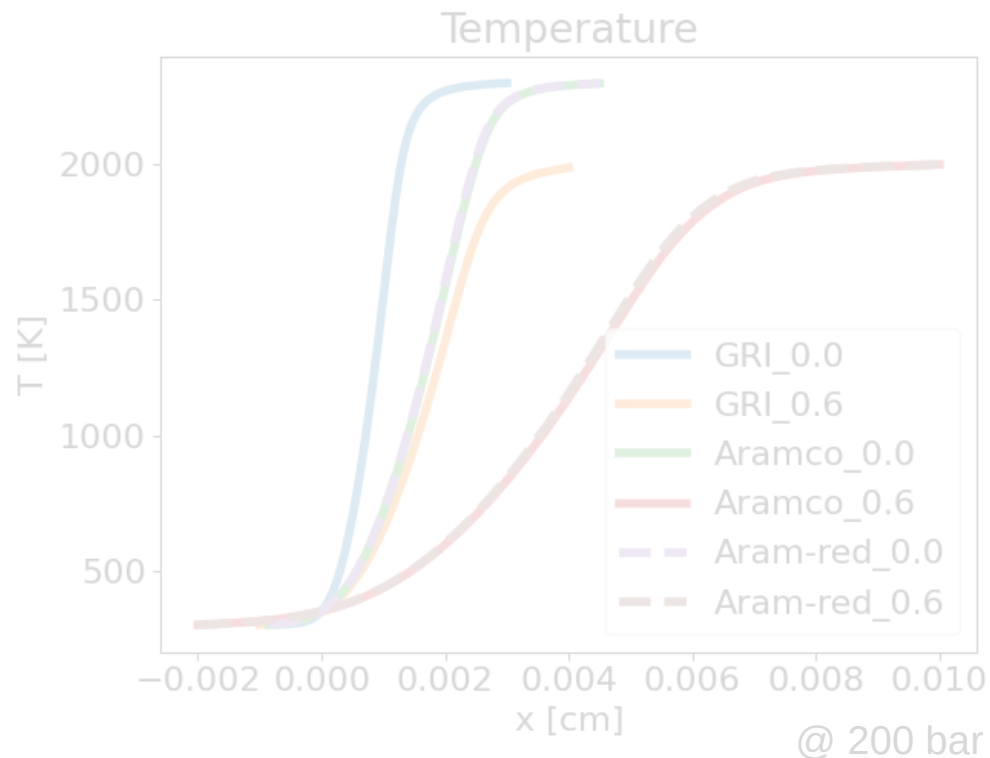
### Validation at low pressure



# One dimensional flames

## Chemistry mechanism

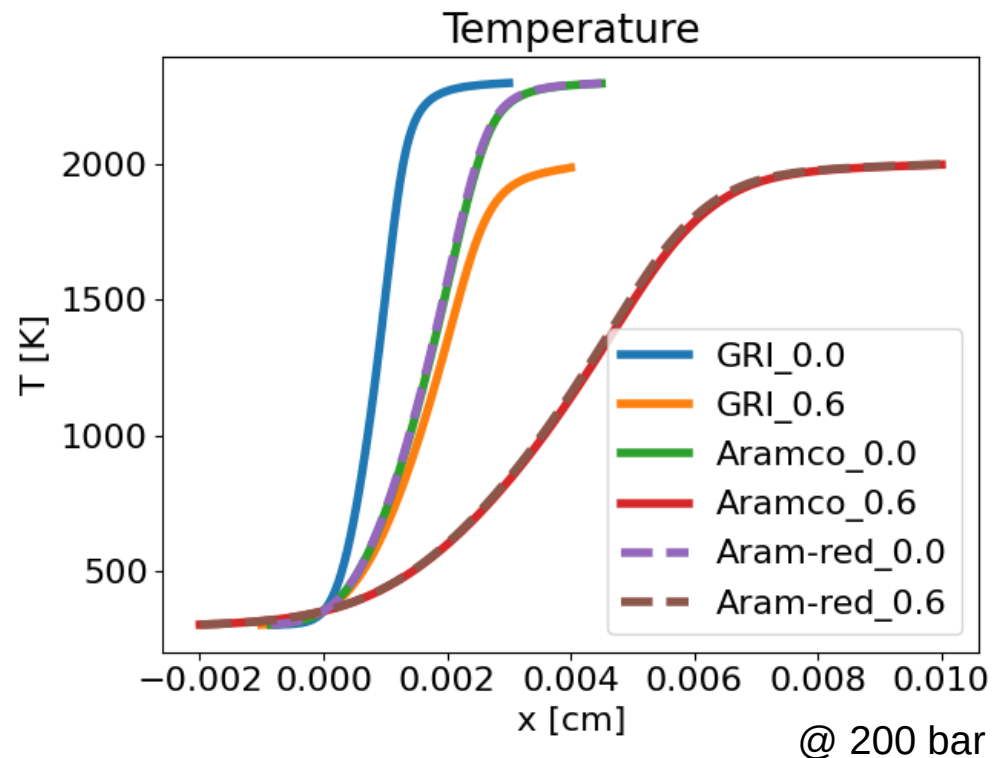
- GRI 3.0 (53 species and 255 reactions, not validated for high p)
- AramcoMech2.0 (493 species and 2716 reactions, computationally expensive)
- AramcoMech2.0 – reduced (37 species and 223 reactions)



# One dimensional flames

## Chemistry mechanism

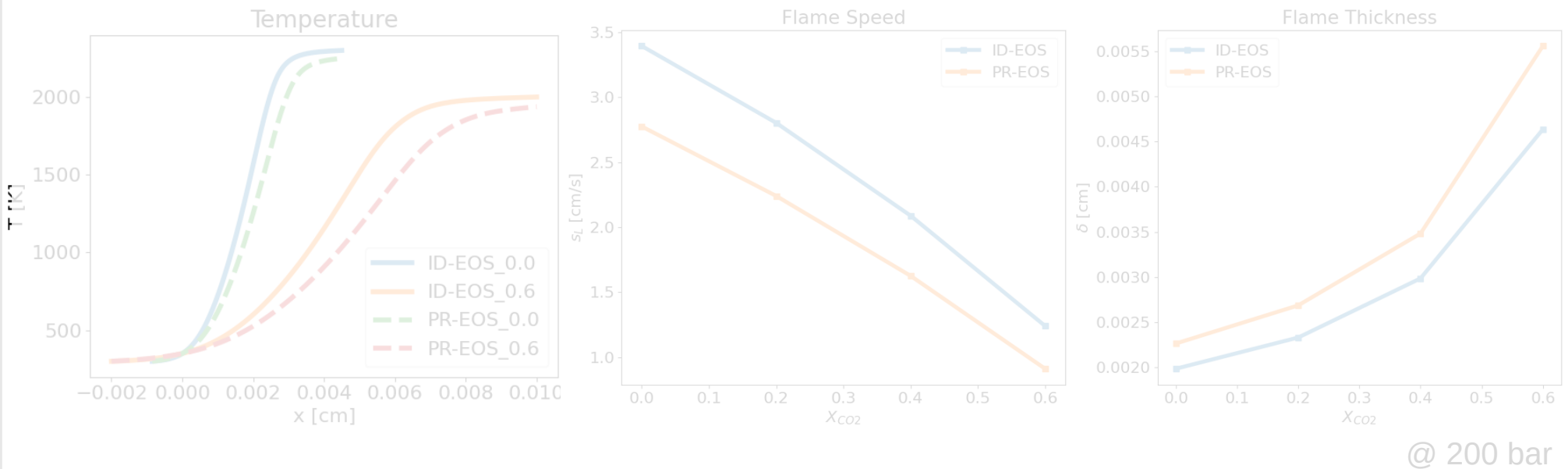
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# One dimensional flames

## EOS, thermodynamics and transport

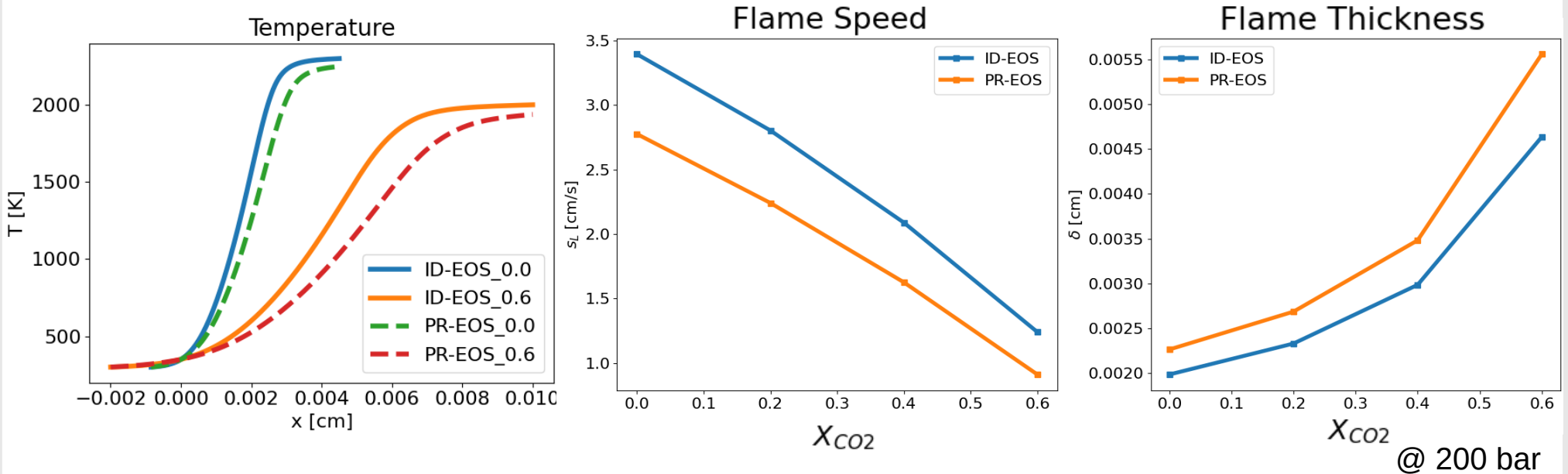
- ID: Ideal Gas EOS, Nasa Polynomials, Power Law
- PR: Peng Robinson EOS, NASA Polynomials + correction, Chung's method



# One dimensional flames

## EOS, thermodynamics and transport

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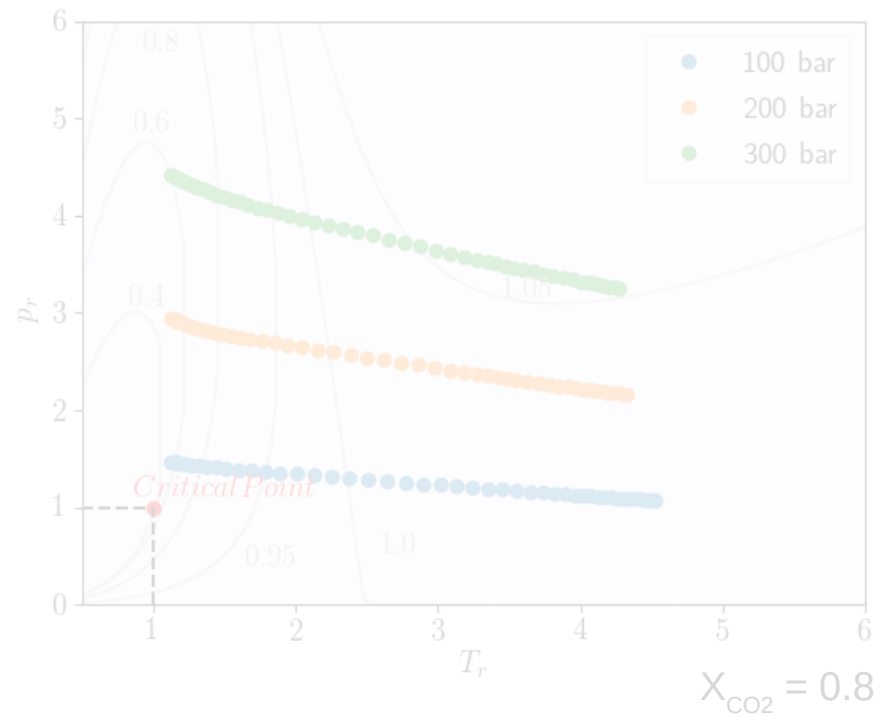
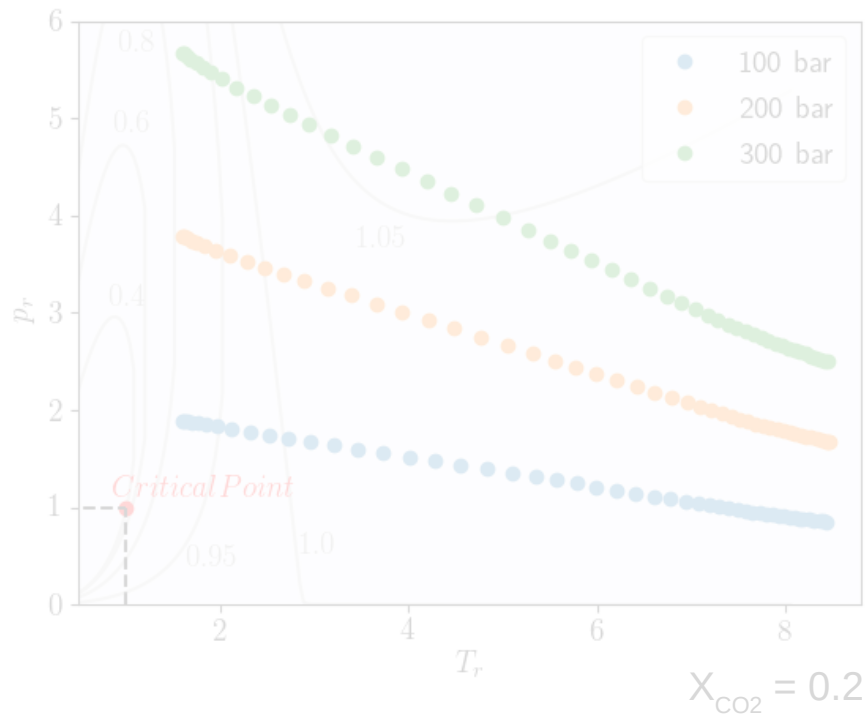


# One dimensional flames

## OxyFuel combustion

	Fuel		Oxidizer	
$\Phi$	CH <sub>4</sub>	CO <sub>2</sub>	O <sub>2</sub>	
1.0	1.0	0.2	0.8	
1.0	1.0	0.4	0.6	
1.0	1.0	0.6	0.4	
1.0	1.0	0.8	0.2	

Unburnt mixture T=300K

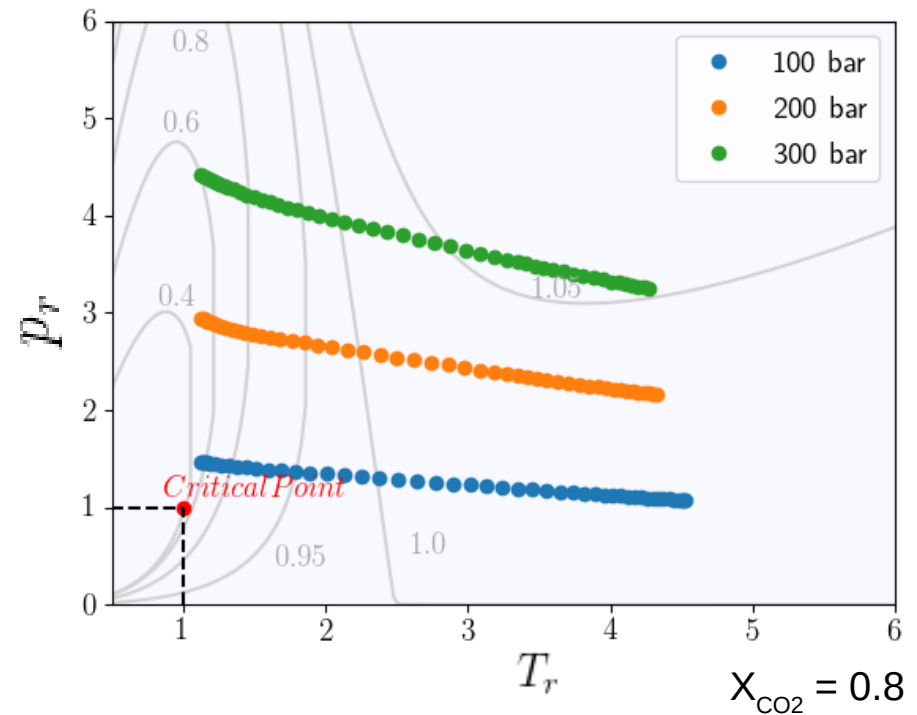
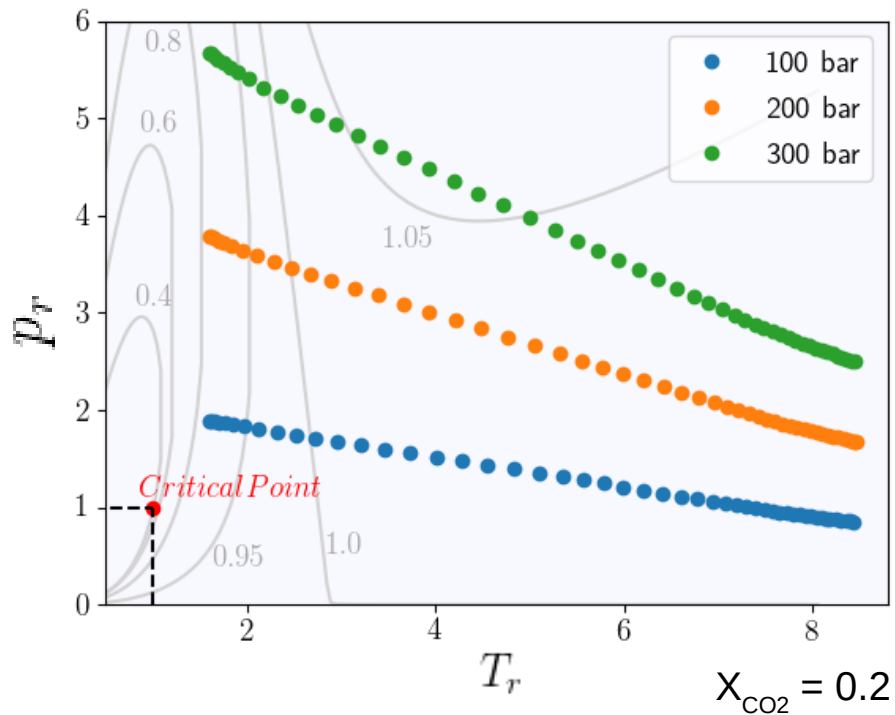


# One dimensional flames

## OxyFuel combustion

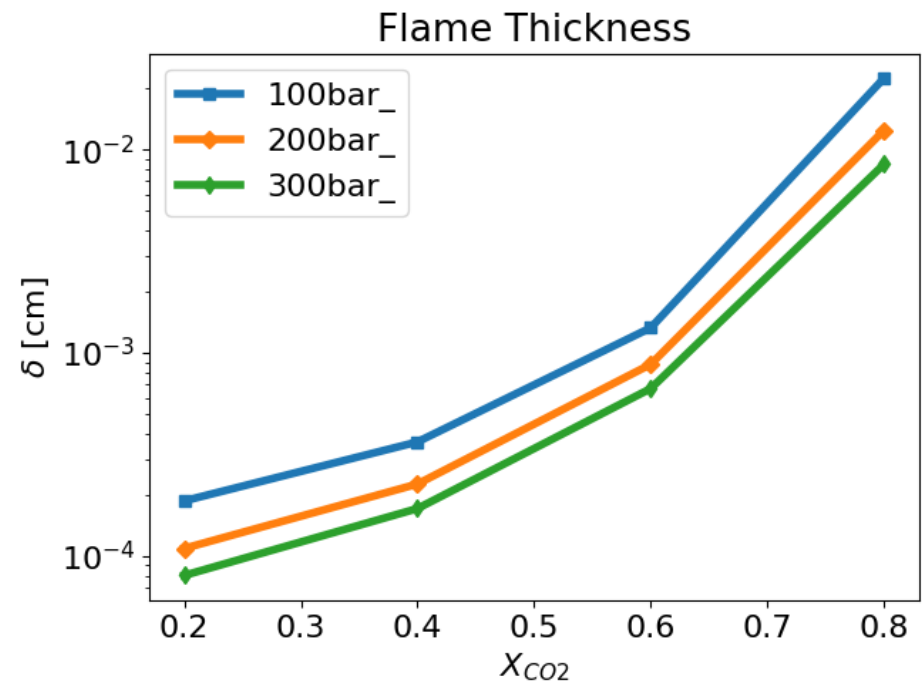
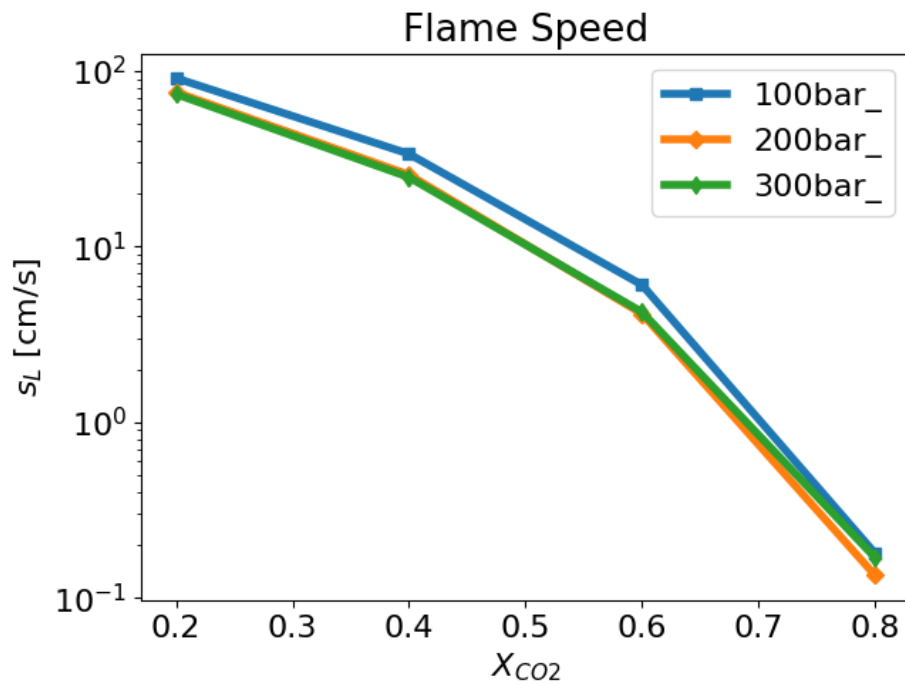
	Fuel		Oxidizer	
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1.0	1.0	0.2	0.8	
1.0	1.0	0.4	0.6	
1.0	1.0	0.6	0.4	
1.0	1.0	0.8	0.2	

Unburnt mixture T=300K



# One dimensional flames

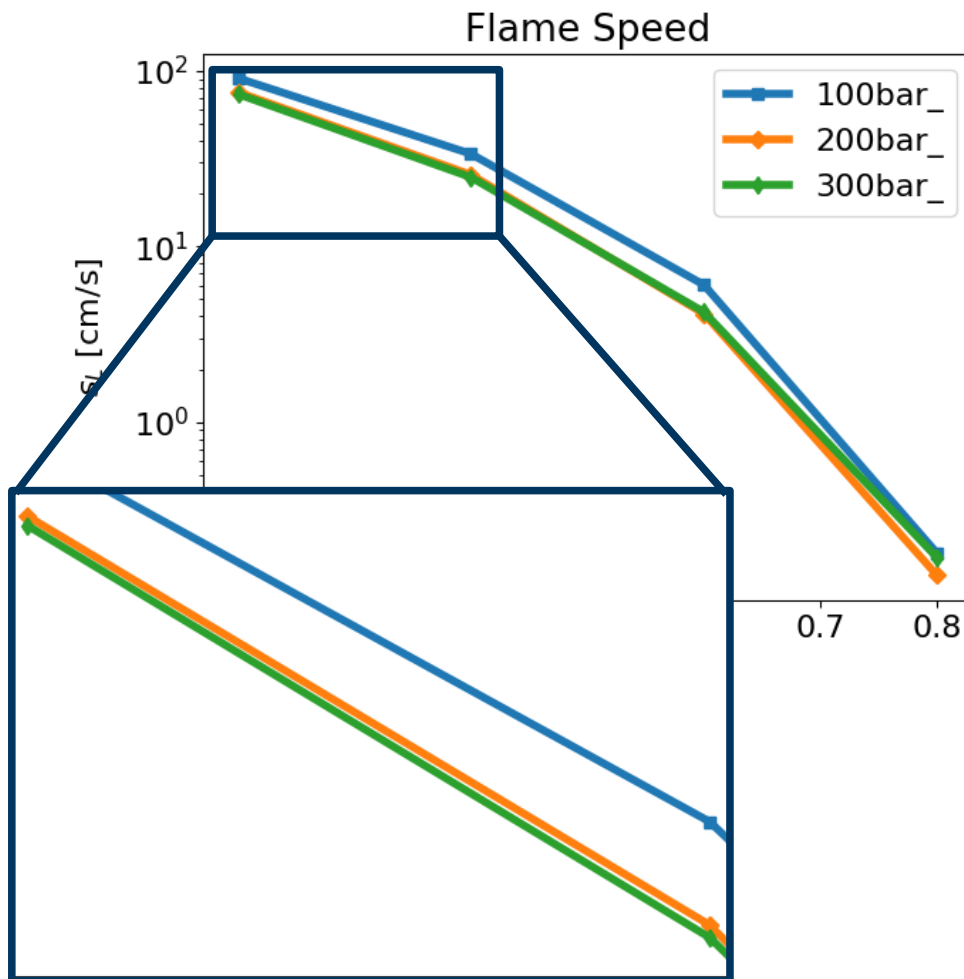
## OxyFuel combustion





# One dimensional flames

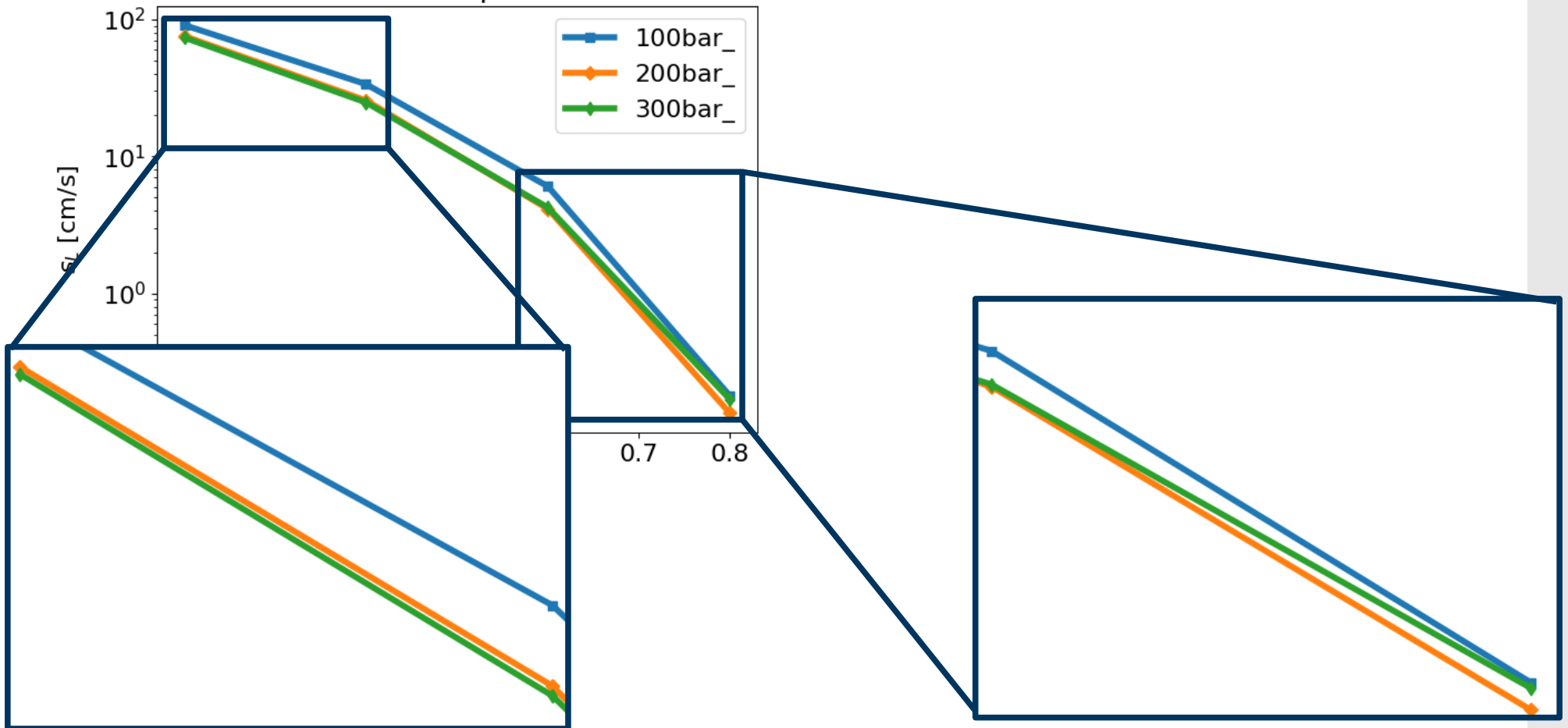
## OxyFuel combustion



# One dimensional flames

## OxyFuel combustion

Flame Speed

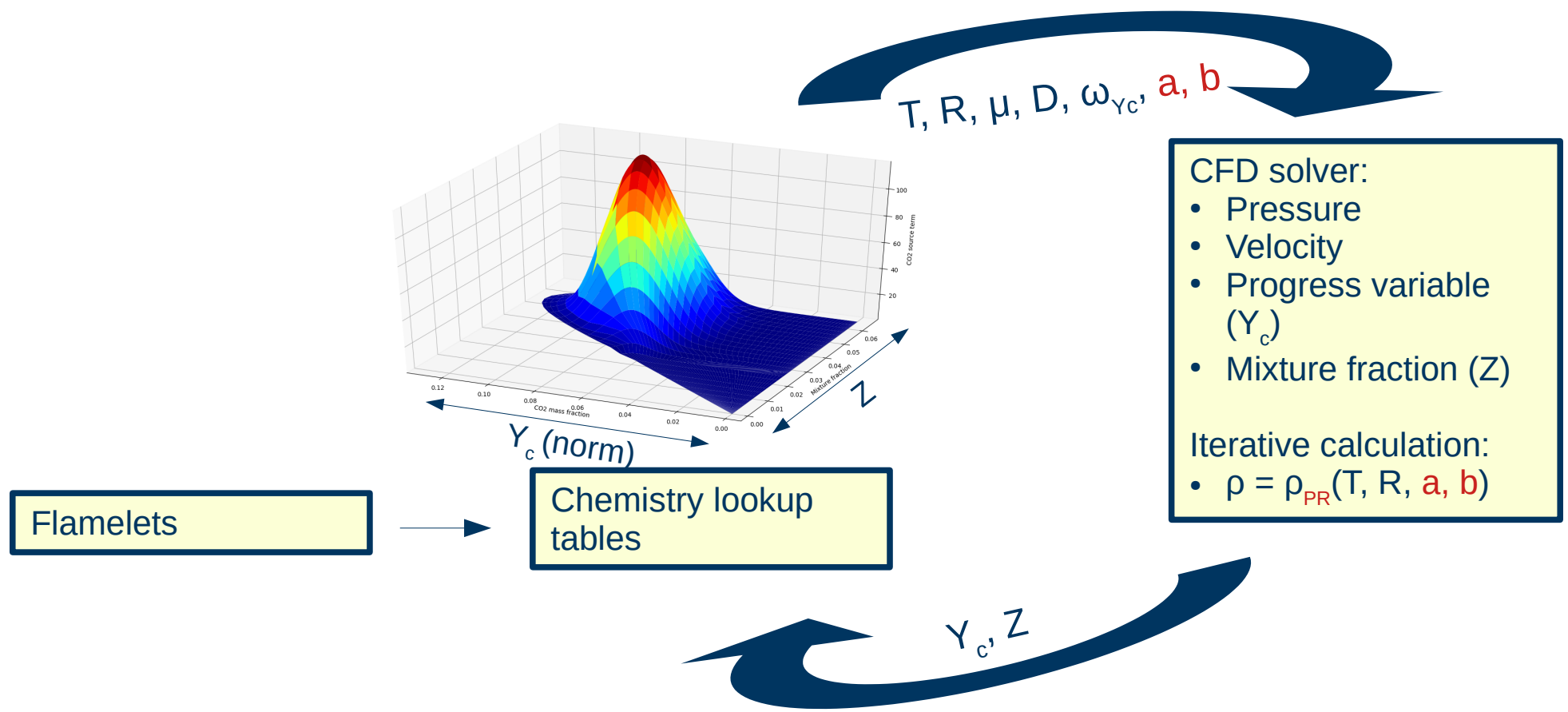


# Outline

- Introduction and Motivation
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- Conclusions and outlook

# Two dimensional flames

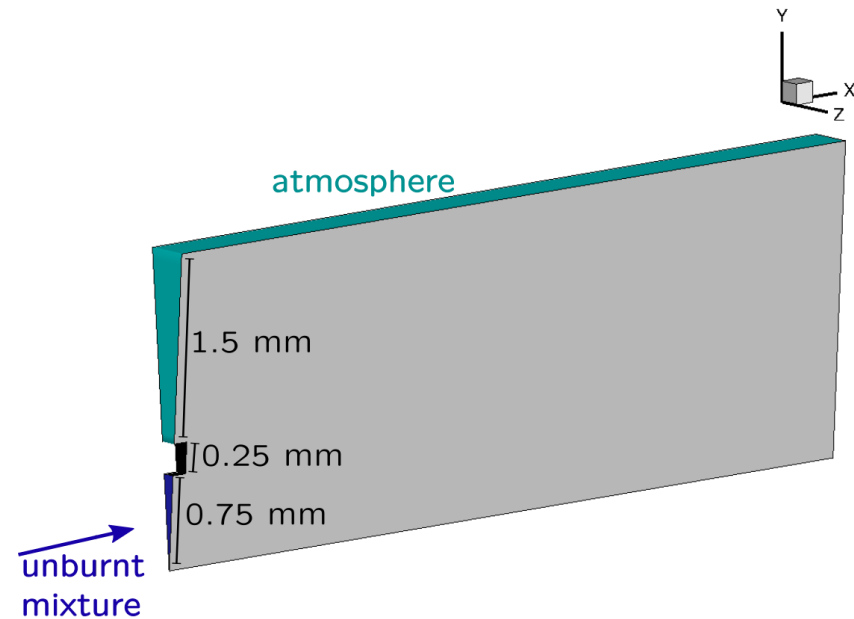
## Coupling CFD solver with chemistry tables



# Two dimensional flames

## Results

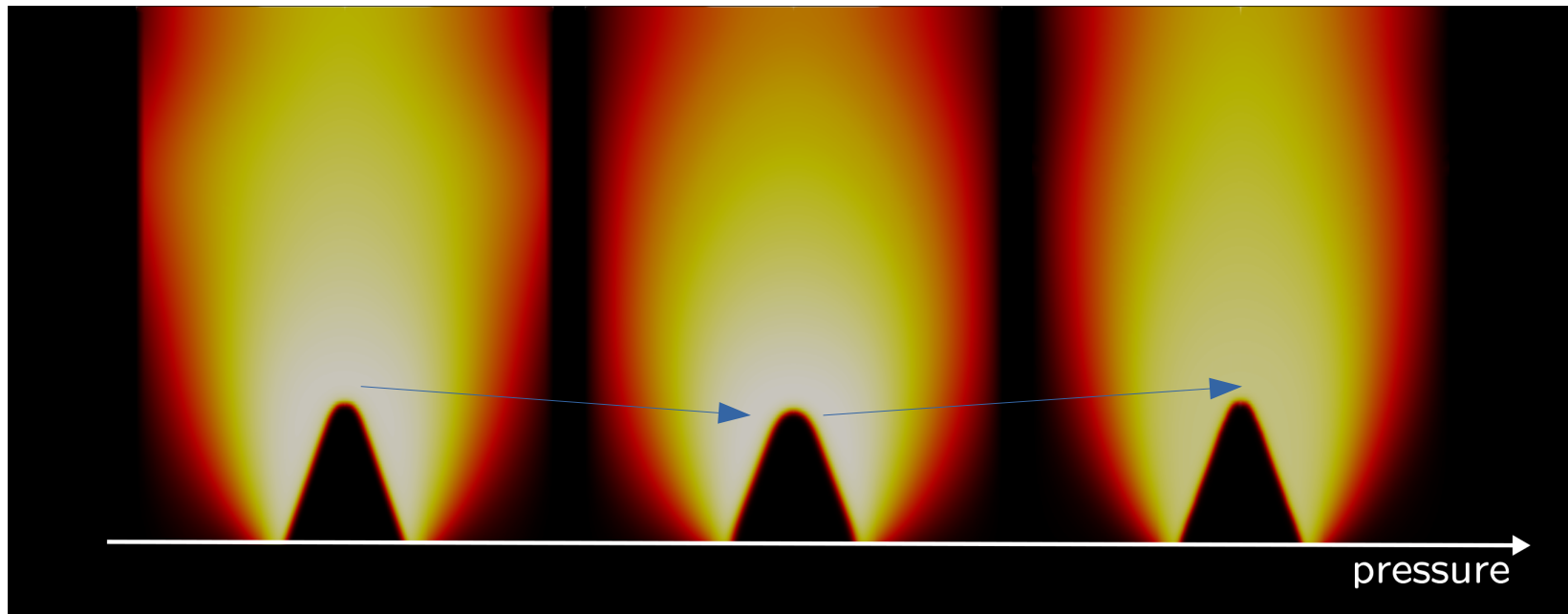
- OpenFOAM + CHEM1D tables
- Unconfined Bunsen configuration
- Fuel:  $\text{CH}_4$ , Oxidizer: 80%  $\text{CO}_2$ , 20%  $\text{O}_2$
- Pressure: 100/200/300 bar
- $\text{Re} = 47 - 206$



# Two dimensional flames

## Results

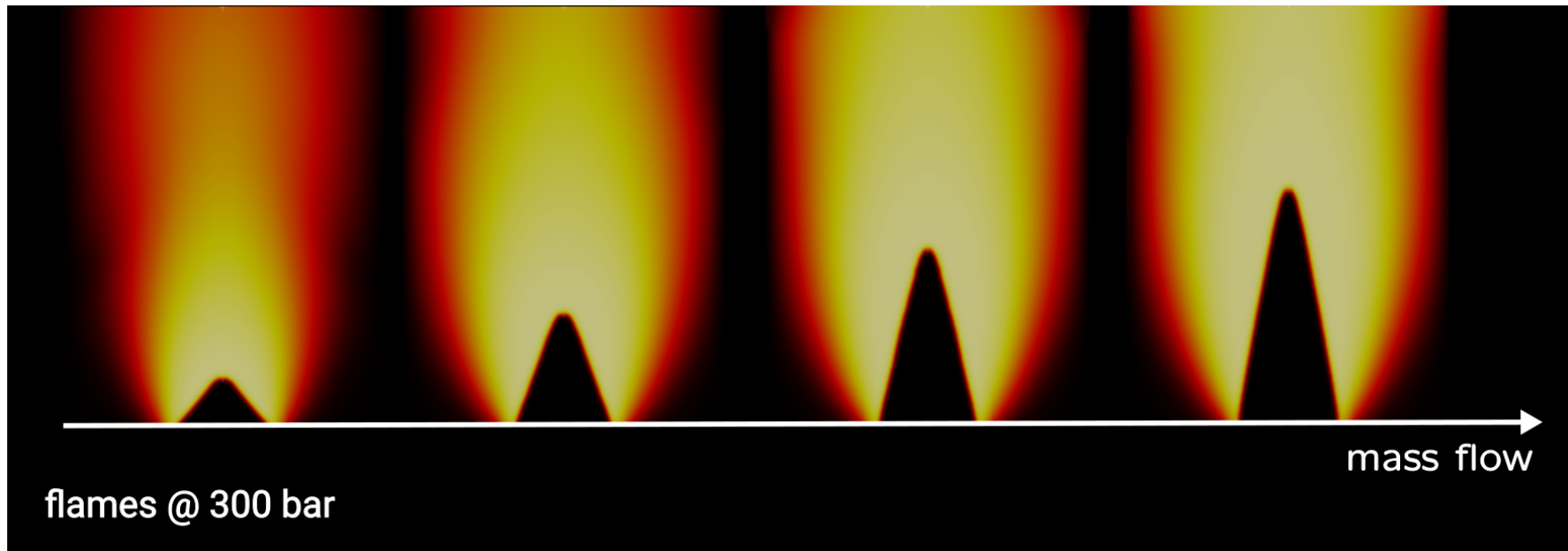
Pressure	Laminar Flame Speed	Unburnt Mixture Velocity
100 bar	1.6926 mm/s	6.7704 mm/s ( $4 s_L$ )
200 bar	1.2691 mm/s	5.0764 mm/s ( $4 s_L$ )
300 bar	1.5988 mm/s	6.3925 mm/s ( $4 s_L$ )



# Two dimensional flames

## Results

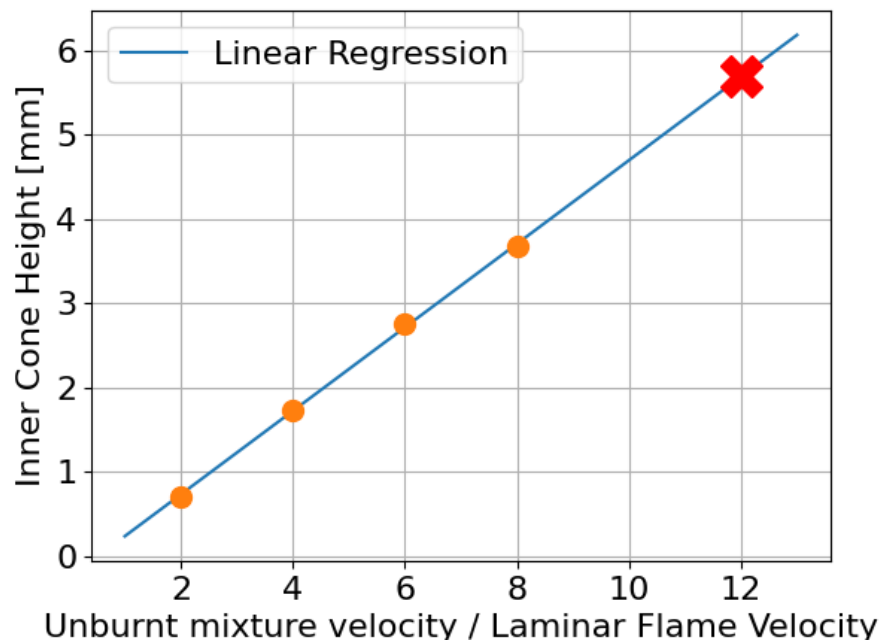
Pressure	Unburnt Mixture Velocity
300 bar	3.1976 mm/s ( $2 s_L$ )
300 bar	6.3925 mm/s ( $4 s_L$ )
300 bar	9.5928 mm/s ( $6 s_L$ )
300 bar	12.7904 mm/s ( $8 s_L$ )
300 bar	19.1856 mm/s ( $12 s_L$ )



# Two dimensional flames

## Results

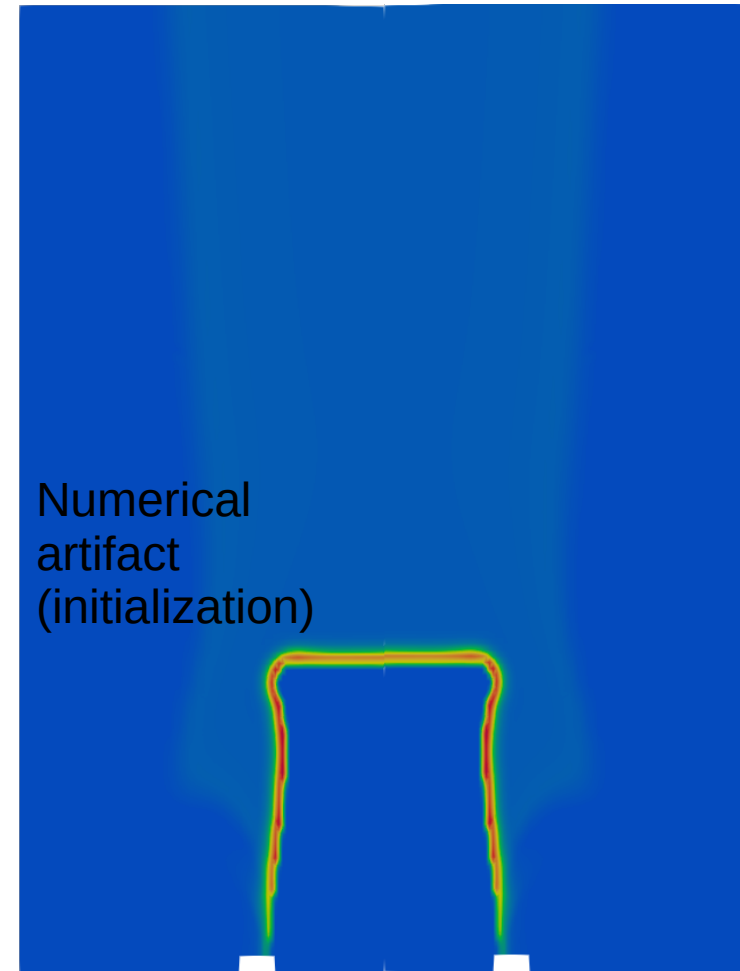
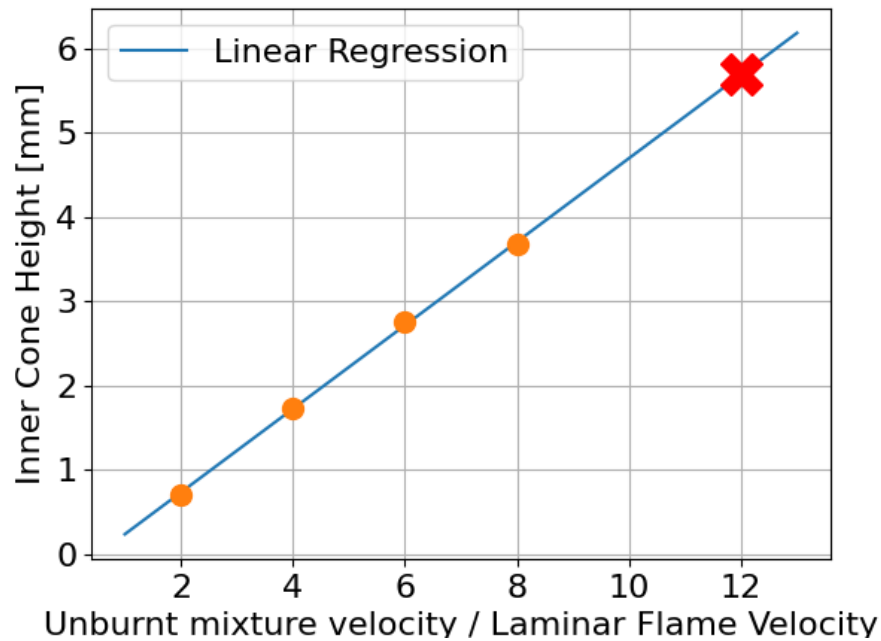
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# Two dimensional flames

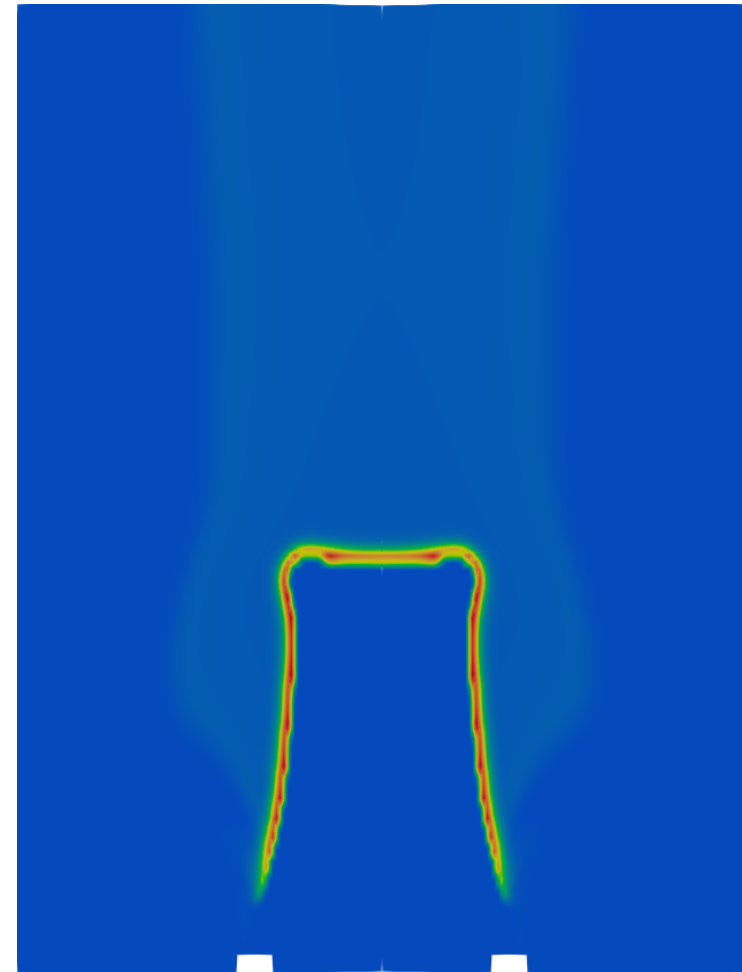
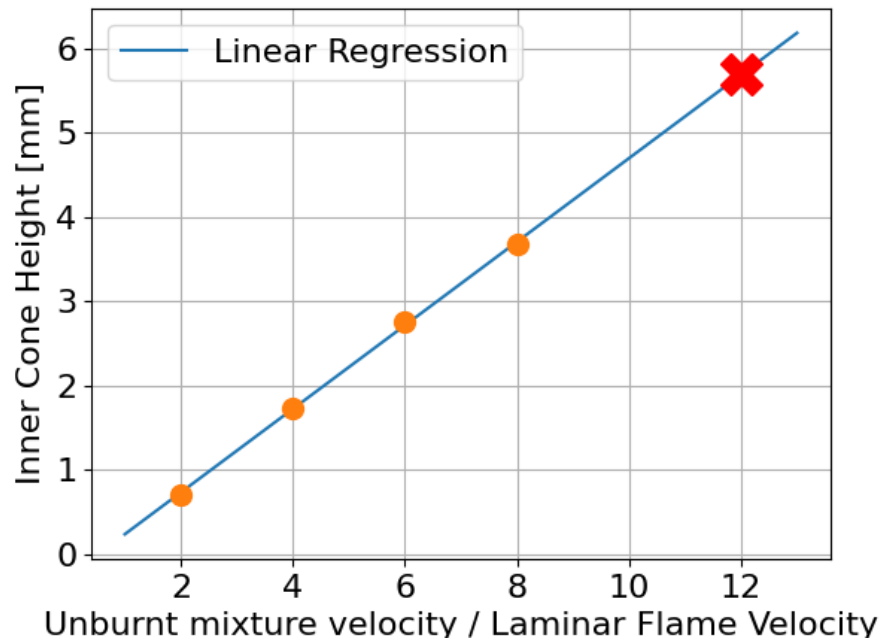
## Results



Progress variable reaction rate  
@  $t = 0.15s$

# Two dimensional flames

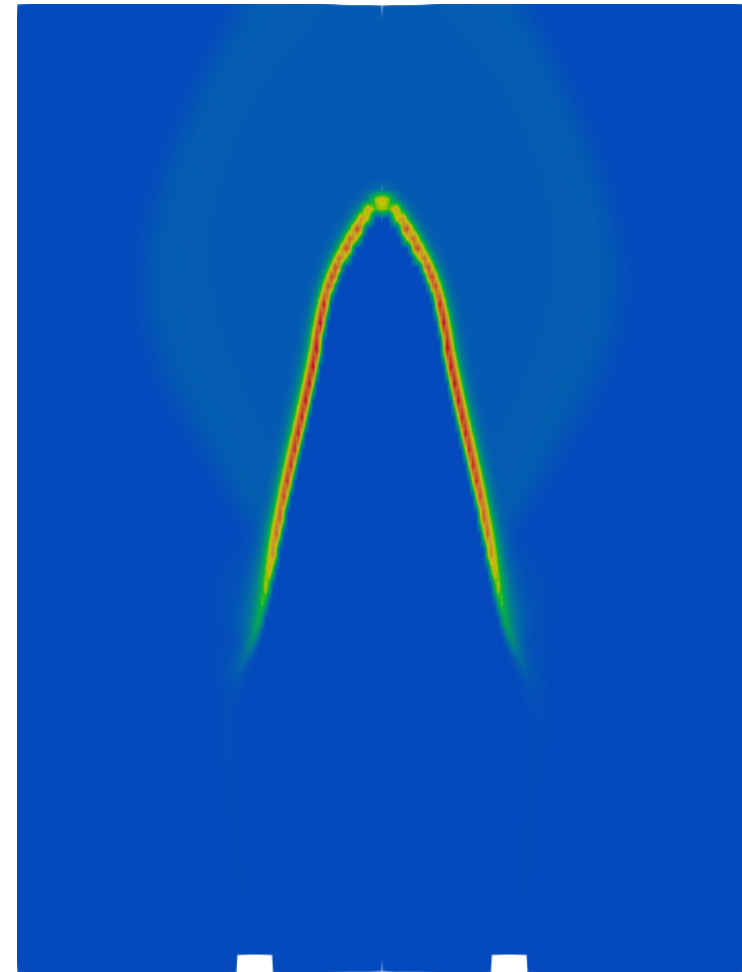
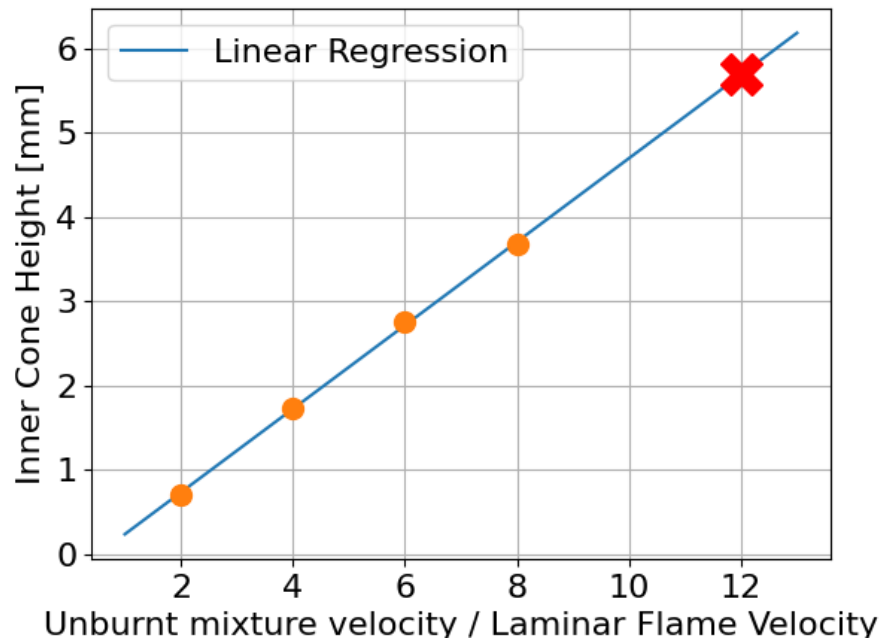
## Results



Progress variable reaction rate  
@ t = 0.20s

# Two dimensional flames

## Results



Progress variable reaction rate  
@  $t = 0.46s$

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- **Conclusions and outlook**

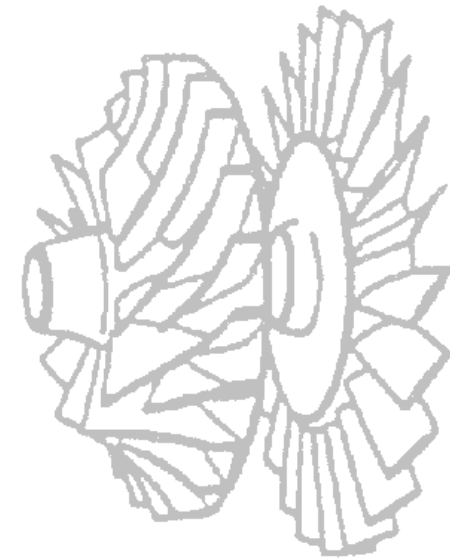
## Conclusions and outlook

- Non ideal equation of state, thermodynamics and transport integrated in detailed chemistry solver
- Reduced detailed chemistry mechanism
- Characterization of 1D premixed flames at very high pressure
- Chemistry lookup tables
- Coupled CFD and detailed chemistry solver taking care of new EOS
- Ongoing study on parameters influencing stability of laminar flames
- Future work:
  - Further validation of results
  - Turbulent flames

# Thank you for your attention.

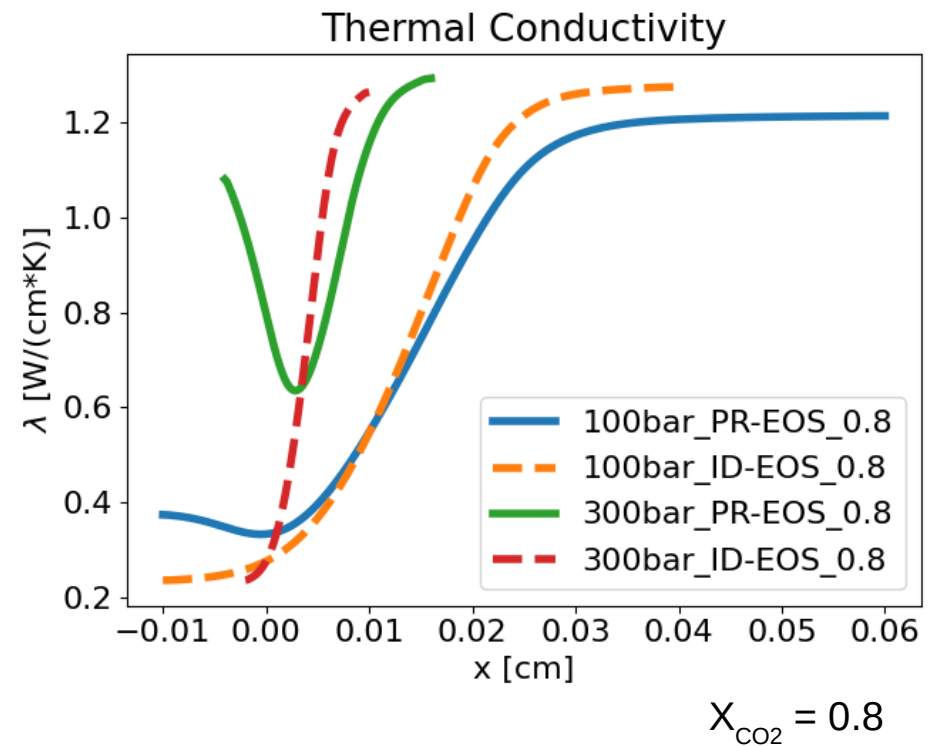
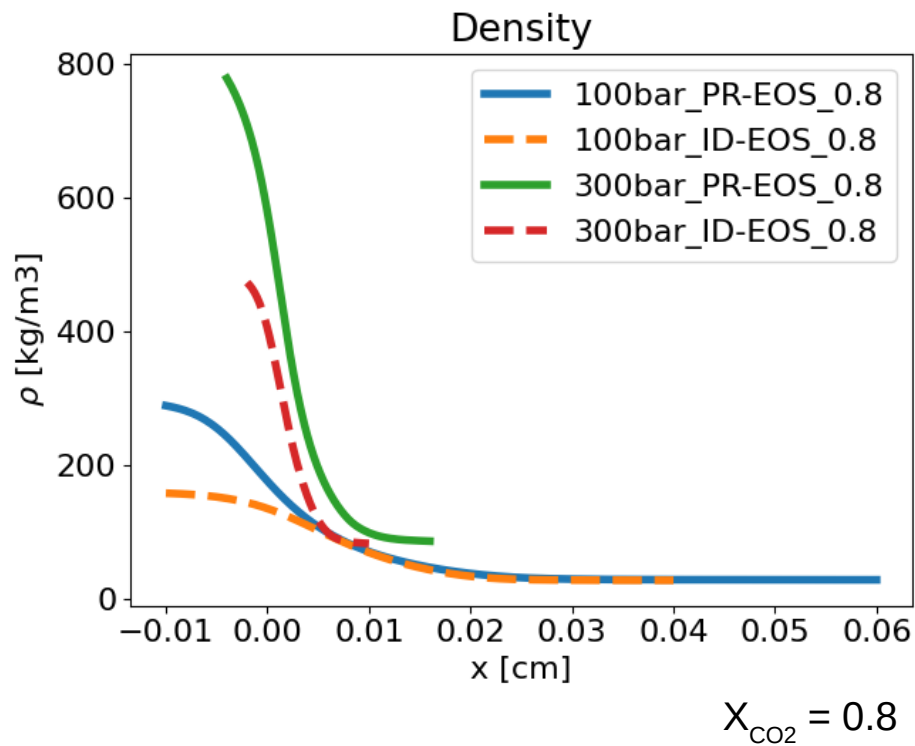
**Federico Lo Presti**

[federico.lopresti@rub.de](mailto:federico.lopresti@rub.de)



# One dimensional flames

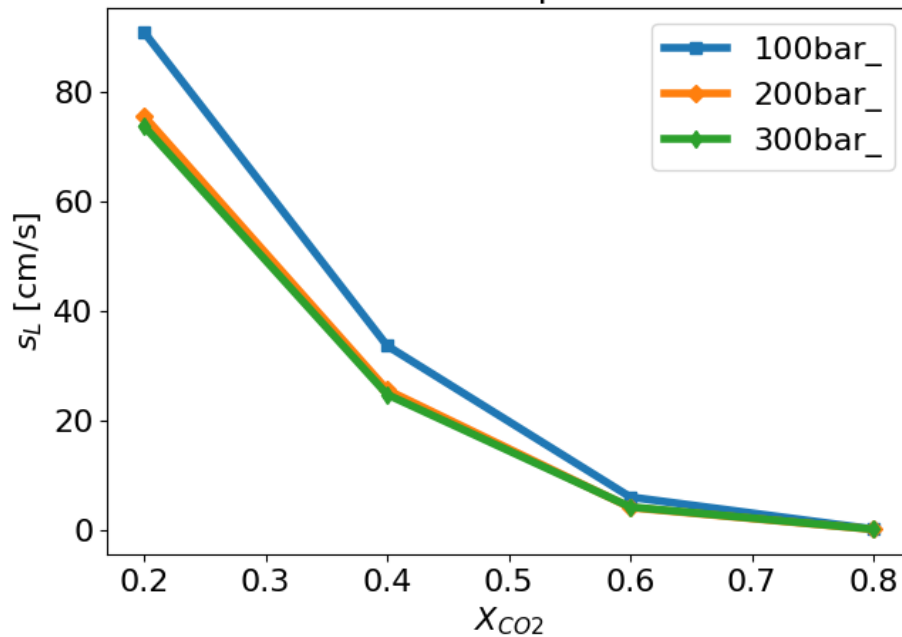
## OxyFuel combustion



# One dimensional flames

## OxyFuel combustion

Flame Speed



Flame Thickness

