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

RUB

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[1], P. Post[1], F. di Mare[1], J. van Oijen[2]

[1] Chair of Thermal Turbomachines and Aeroengines, Ruhr University Bochum

[2] 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

Reduce carbon and pollutant emissions in energy and transport

Ensure affordable and reliable sources of energy, keeping up with incresing demand

?

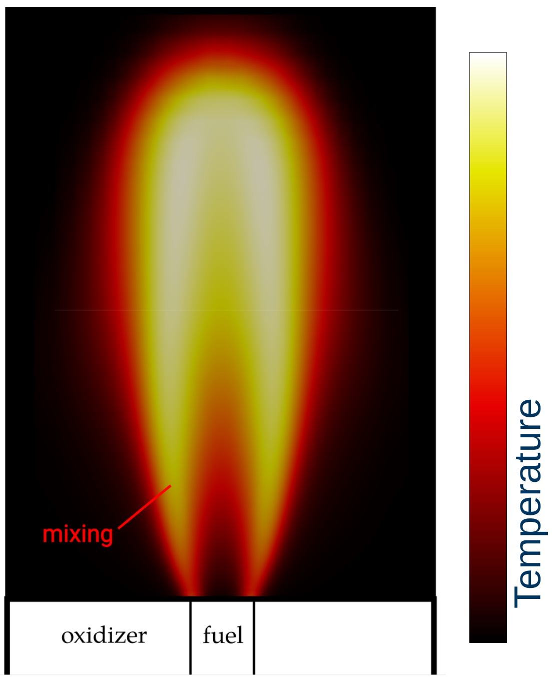
New technological solutions, beyond current standards

Some research trends in gas turbines:

- Hydrogen combustion
- Carbon Capture and Sequestration
  e. g. in directly fired supercritical CO_2 power cycles
  - reduce CO_2 emissions
  - oxyfuel: no NO_x
  - higher density: lower size

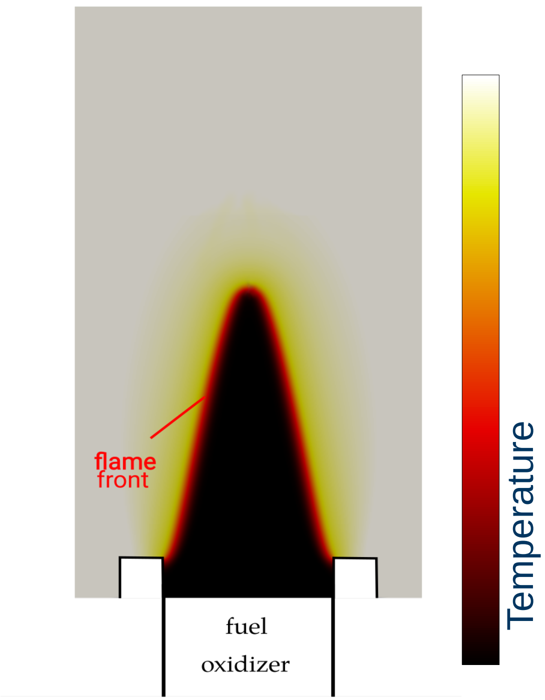
Introduction and motivation

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

- 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

One dimensional flames

Chemistry solver

CHEM1D[1]

- 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

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

One dimensional flames

Biogas mixtures

	Fuel		Oxidizer		
Φ	CH_4	CO_2	N_2	O_2	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

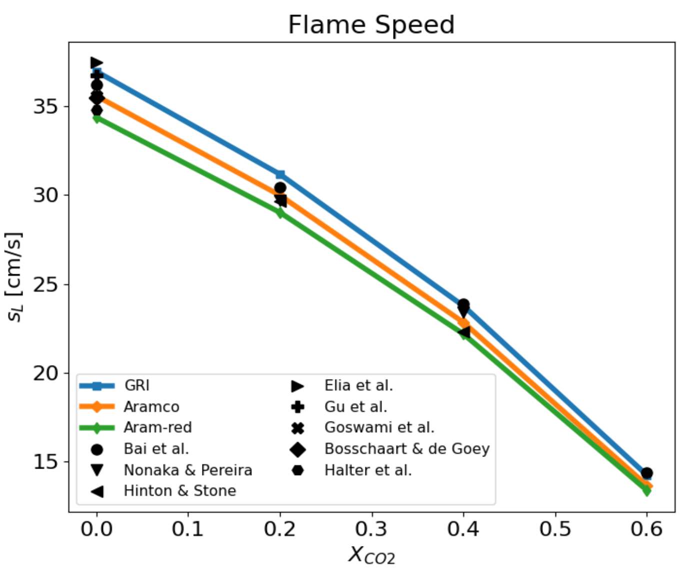
One dimensional flames

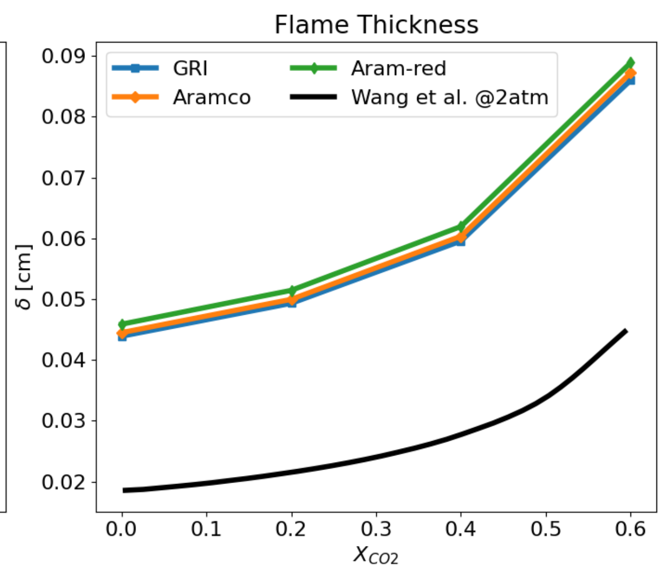
Biogas mixtures

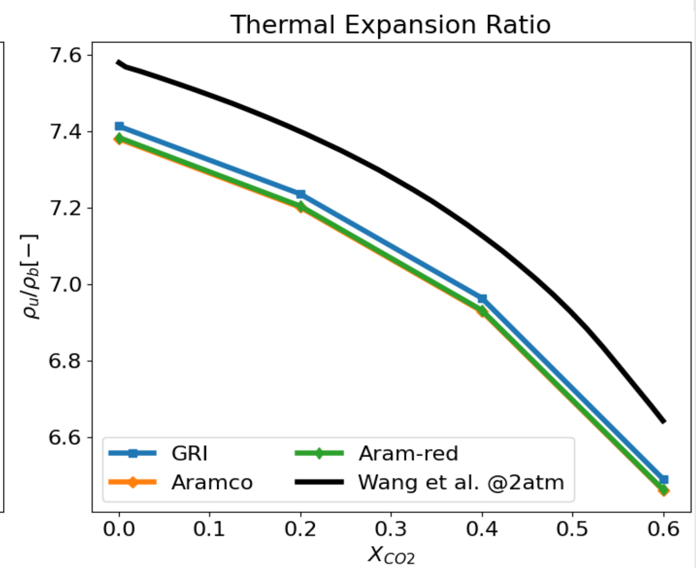
	Fuel			Oxidizer	
Φ	CH_4	CO_2	N_2	O_2	Ar
1.0	1.0	0.0	0.781	0.21	0.009
1.0	0.8	0.2	0.781	0.21	0.009
1.0	0.6	0.4	0.781	0.21	0.009
1.0	0.4	0.6	0.781	0.21	0.009

Unburnt mixture T=300K

Validation at low pressure







One dimensional flames

Chemistry mechanism

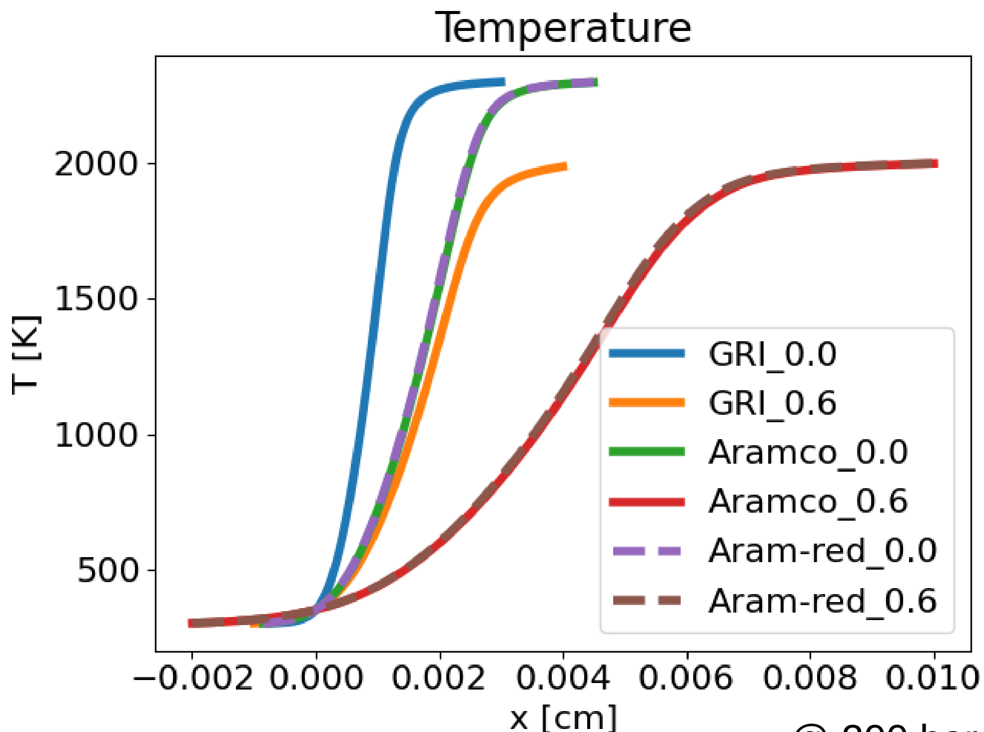
- GRI 3.0 (53 species and 255 reactions, not validated for high p)
- AramcoMech2.0 (493 species and 2716 reactions, computationally expensive)
- AramcoMech2.0 – reduced (37 species and 223 reactions)

@ 200 bar

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)



@ 200 bar

One dimensional flames

EOS, thermodynamics and transport

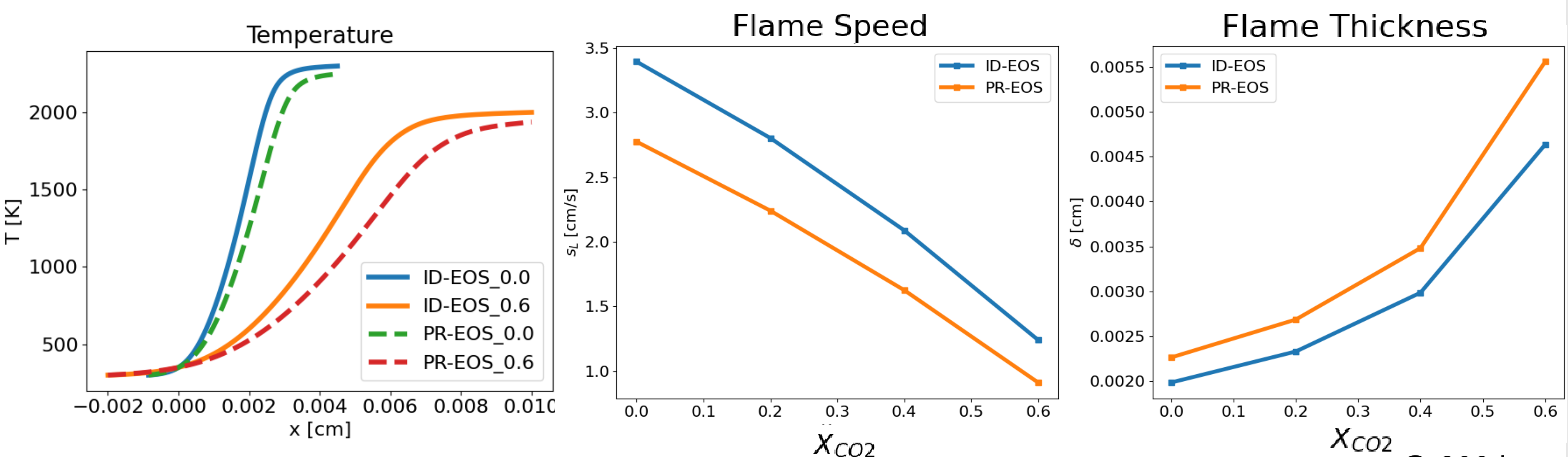
- ID: Ideal Gas EOS, Nasa Polynomials, Power Law
- PR: Peng Robinson EOS, NASA Polynomials + correction, Chung's method

@ 200 bar

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



@ 200 bar

One dimensional flames

OxyFuel combustion

	Fuel	Oxidizer	
Φ	**CH_4**	**CO_2**	**O_2**
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

X_{CO2} = 0.2

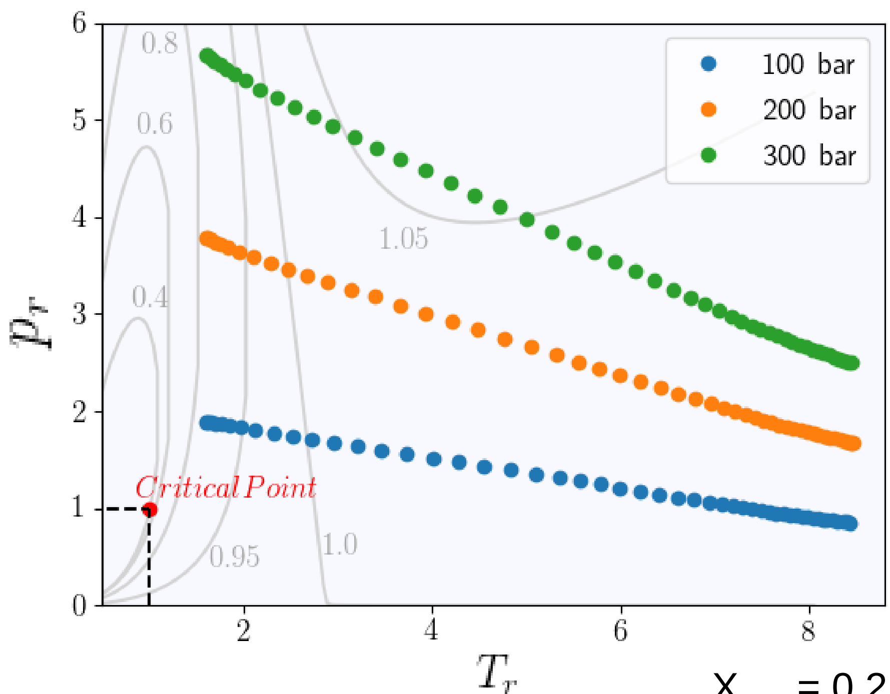
X_{CO2} = 0.8

One dimensional flames

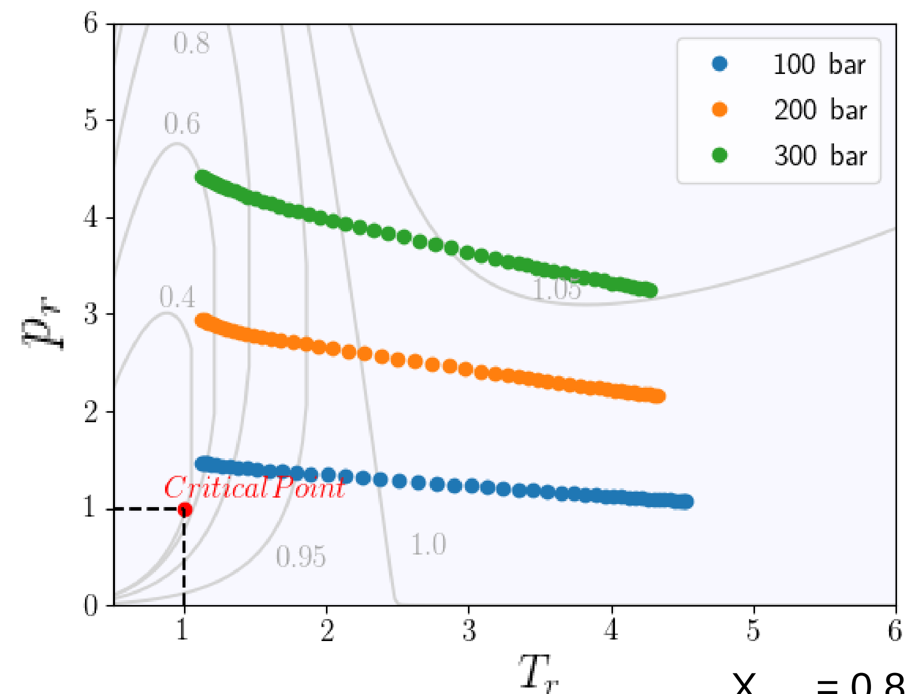
OxyFuel combustion

	Fuel	Oxidizer	
Φ	**CH_4**	**CO_2**	**O_2**
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



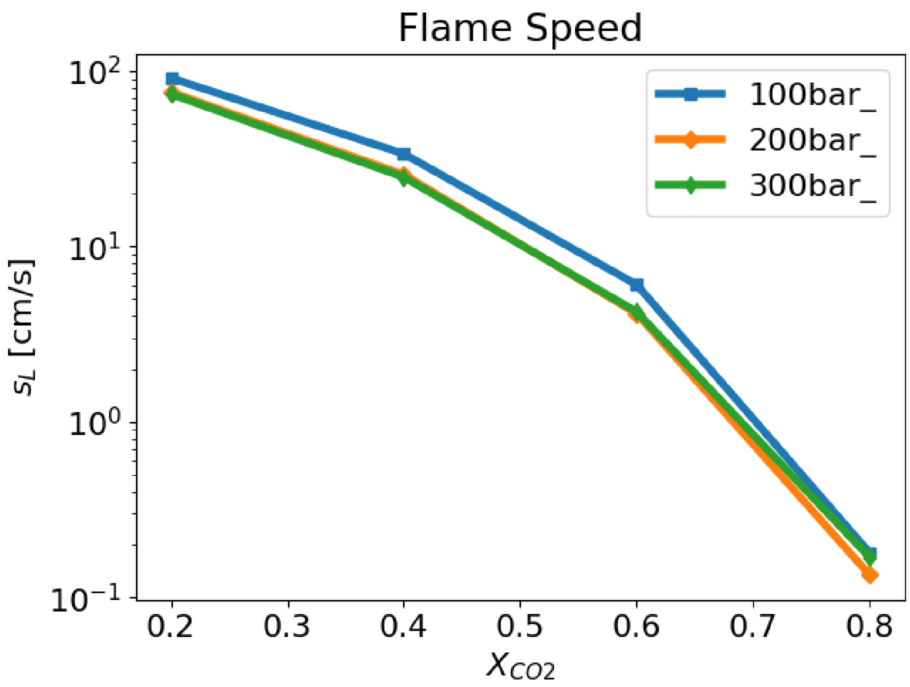
X_{CO2} = 0.2

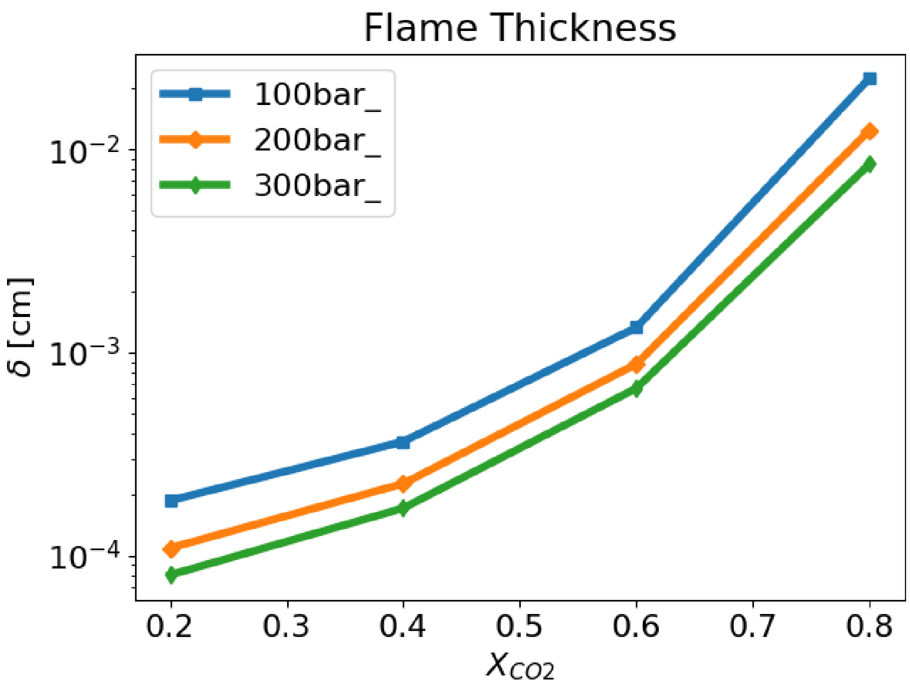


X_{CO2} = 0.8

One dimensional flames

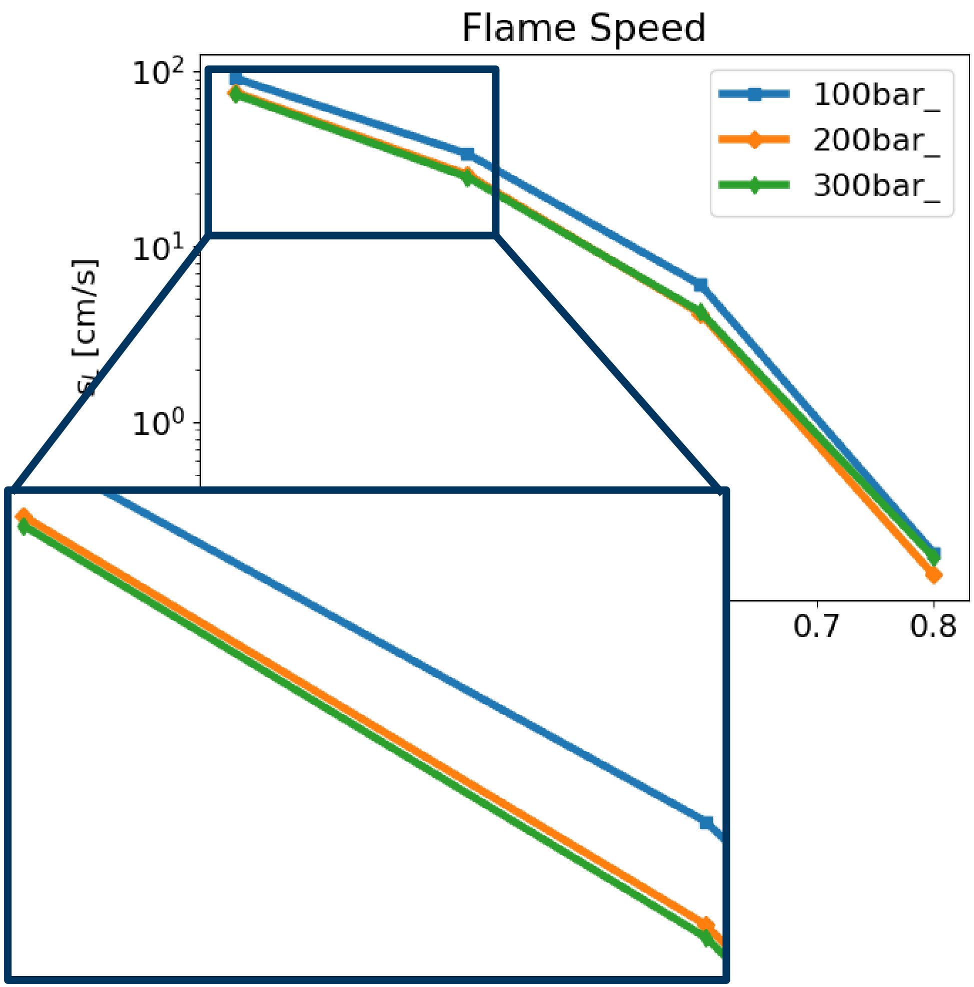
OxyFuel combustion





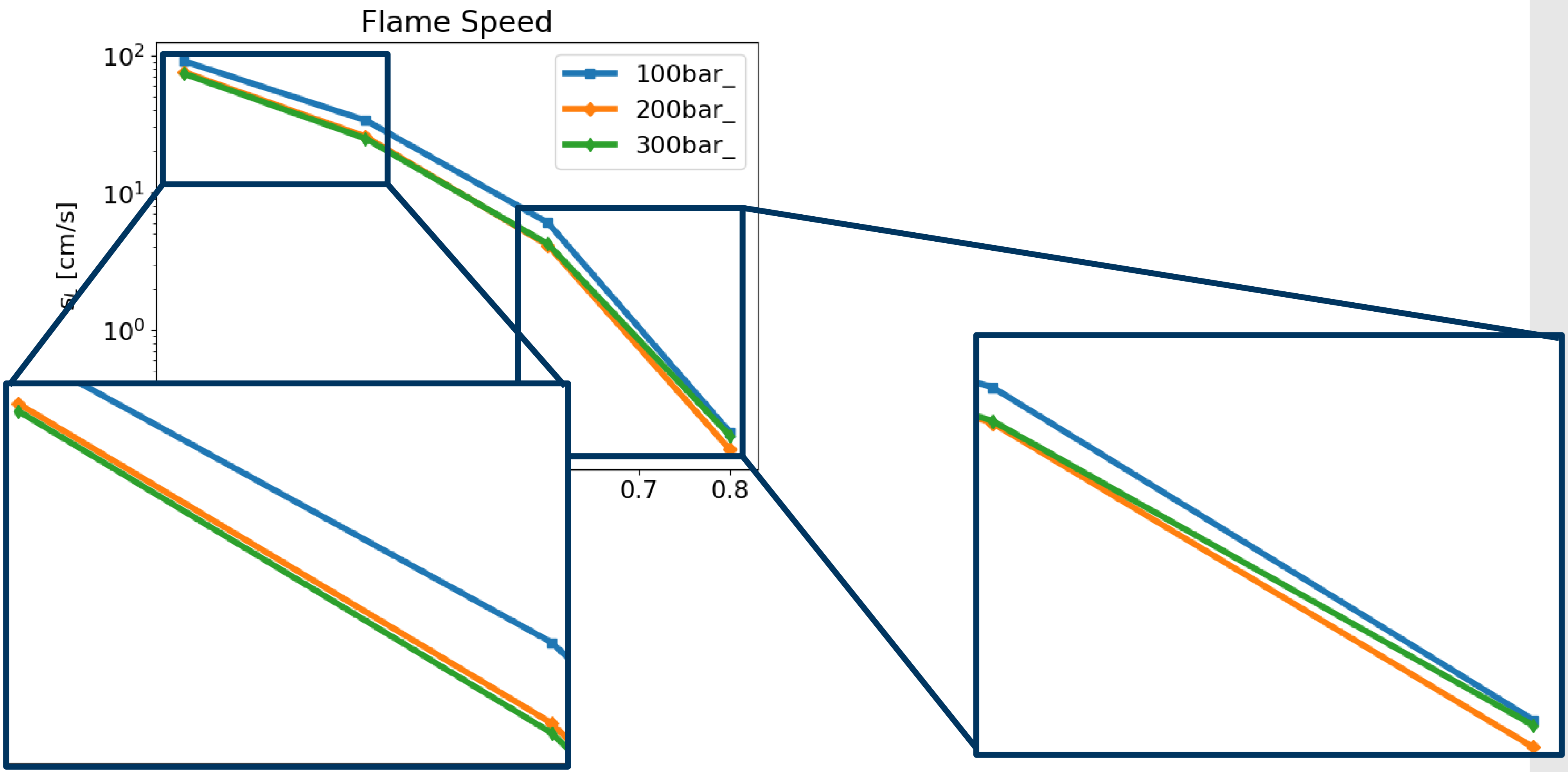
One dimensional flames

OxyFuel combustion



One dimensional flames

OxyFuel combustion



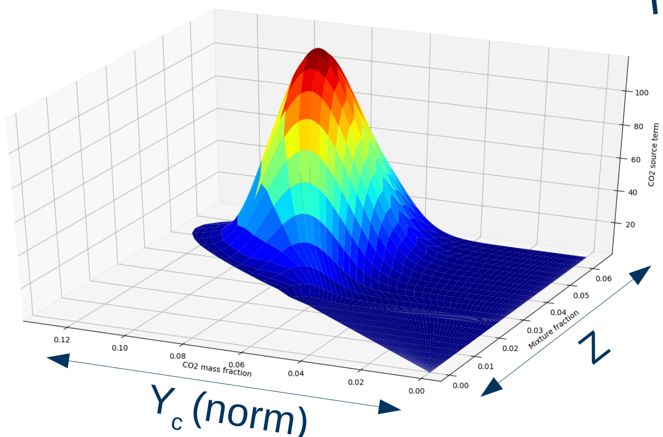
Outline

- 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

Two dimensional flames

Coupling CFD solver with chemistry tables

$T, R, \mu, D, \omega_{Yc}$, a, b



Flamelets → Chemistry lookup tables

CFD solver:
- Pressure
- Velocity
- Progress variable (Y_c)
- Mixture fraction (Z)

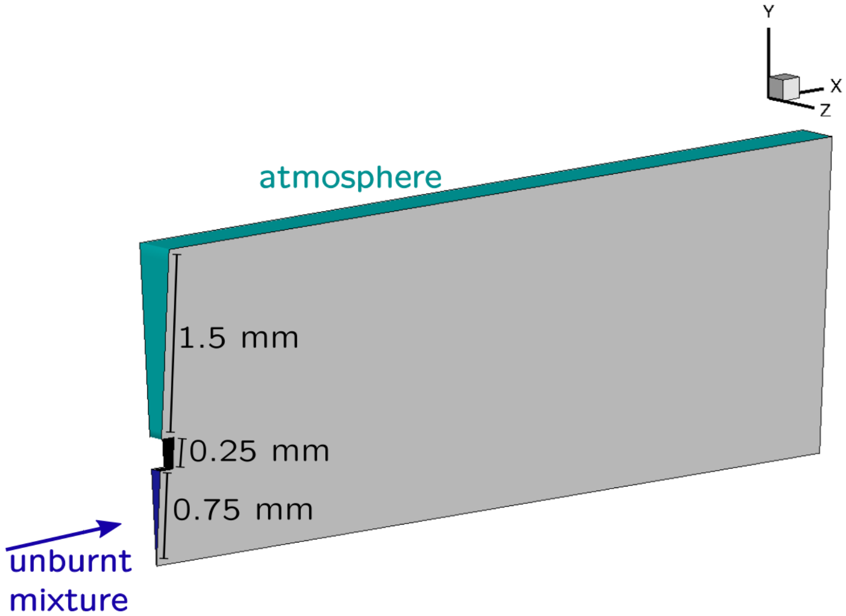
Iterative calculation:
- $\rho = \rho_{PR}(T, R, a, b)$

Y_c, Z

Two dimensional flames

Results

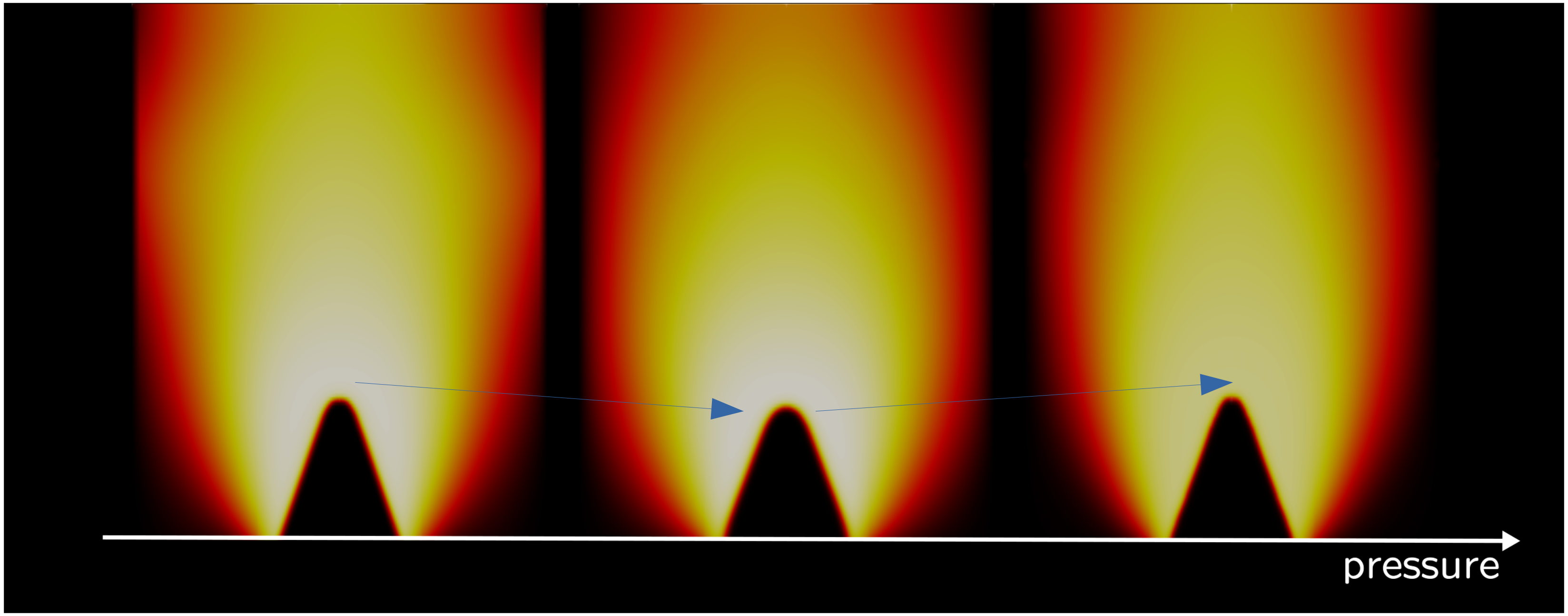
- OpenFOAM + CHEM1D tables
- Unconfined Bunsen configuration
- Fuel: CH_4, Oxidizer: 80% CO_2, 20% O_2
- Pressure: 100/200/300 bar
- Re = 47 - 206



Two dimensional flames

Results

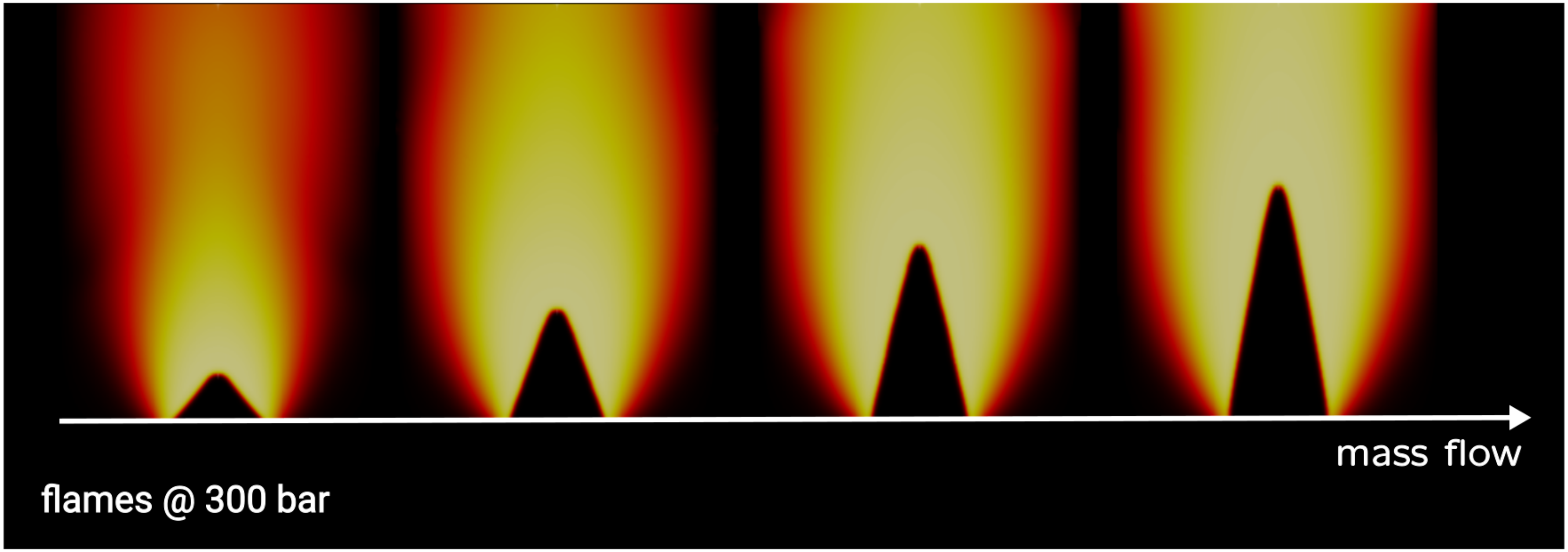
Pressure	Laminar Flame Speed	Unburnt Mixture Velocity
100 bar	1.6926 mm/s	6.7704 mm/s (4 s_L)
200 bar	1.2691 mm/s	5.0764 mm/s (4 s_L)
300 bar	1.5988 mm/s	6.3925 mm/s (4 s_L)



Two dimensional flames

Results

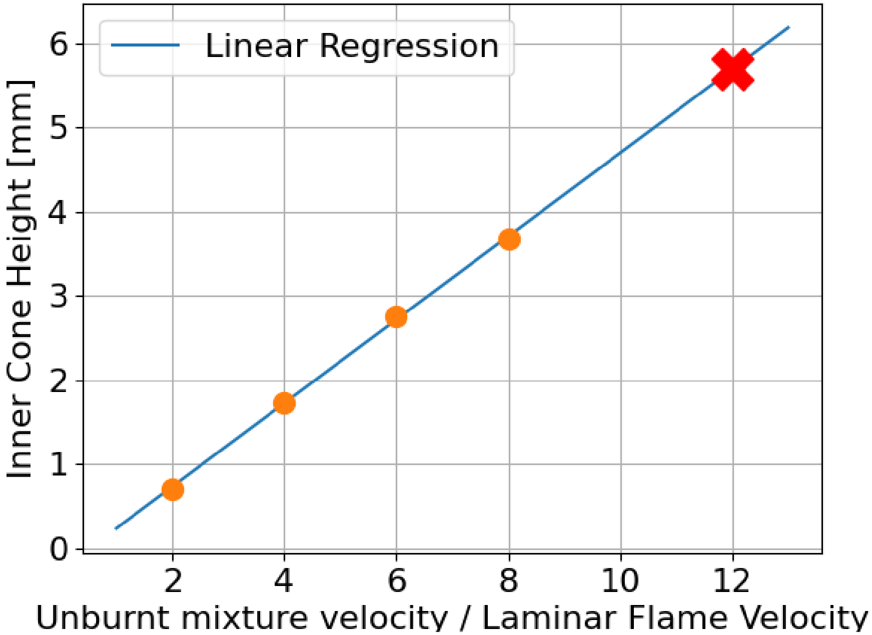
Pressure	Unburnt Mixture Velocity
300 bar	3.1976 mm/s (2 s_L)
300 bar	6.3925 mm/s (4 s_L)
300 bar	9.5928 mm/s (6 s_L)
300 bar	12.7904 mm/s (8 s_L)
300 bar	19.1856 mm/s (12 s_L)



Two dimensional flames

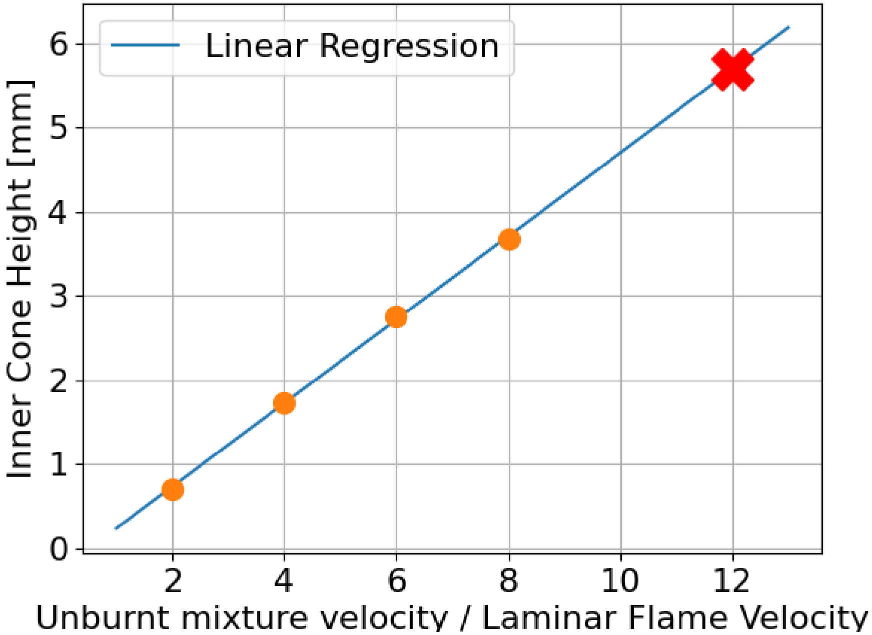
Results

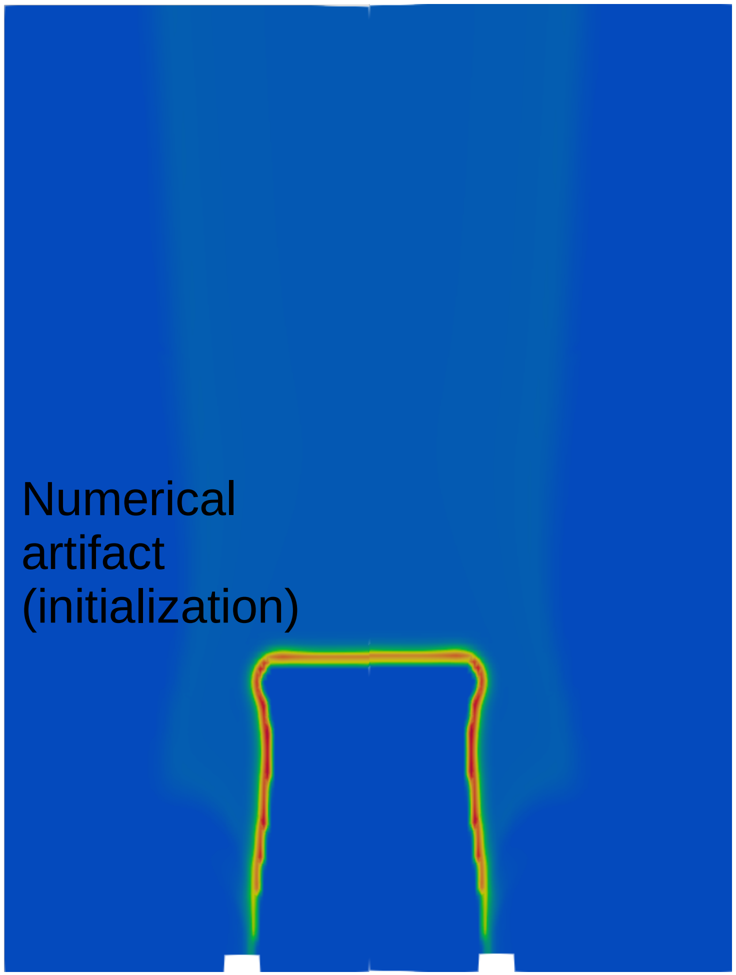
Pressure	Unburnt Mixture Velocity
300 bar	3.1976 mm/s (2 s_L)
300 bar	6.3925 mm/s (4 s_L)
300 bar	9.5928 mm/s (6 s_L)
300 bar	12.7904 mm/s (8 s_L)
300 bar	19.1856 mm/s (12 s_L)



Two dimensional flames

Results

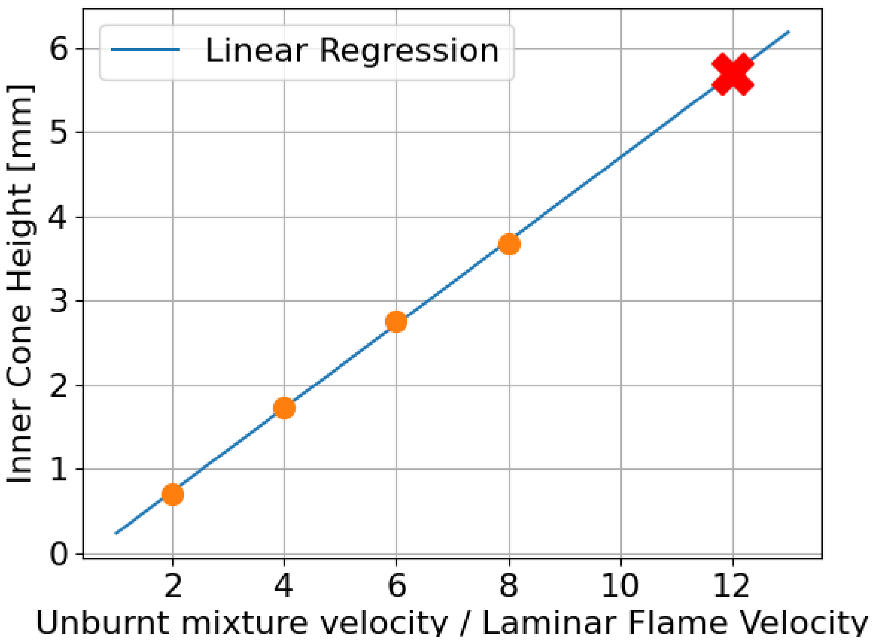


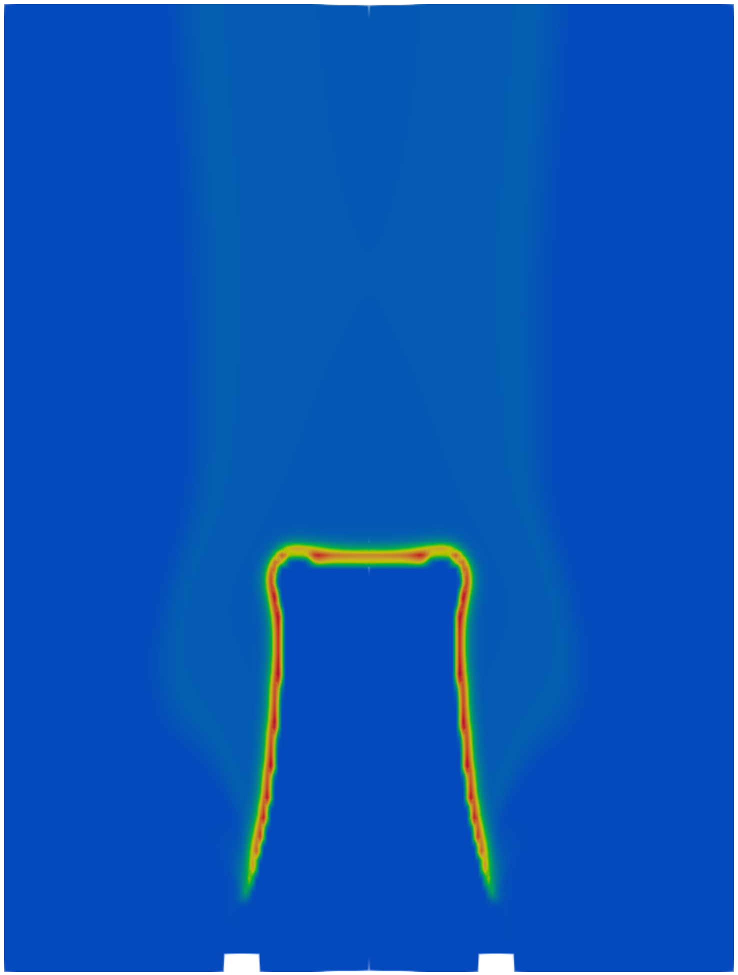


Progress variable reaction rate @ t = 0.15s

Two dimensional flames

Results

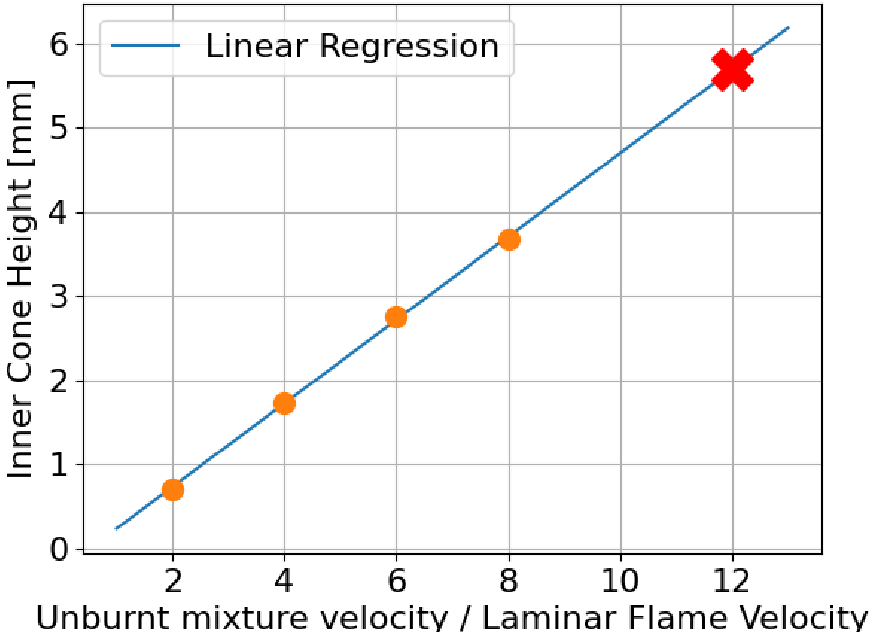


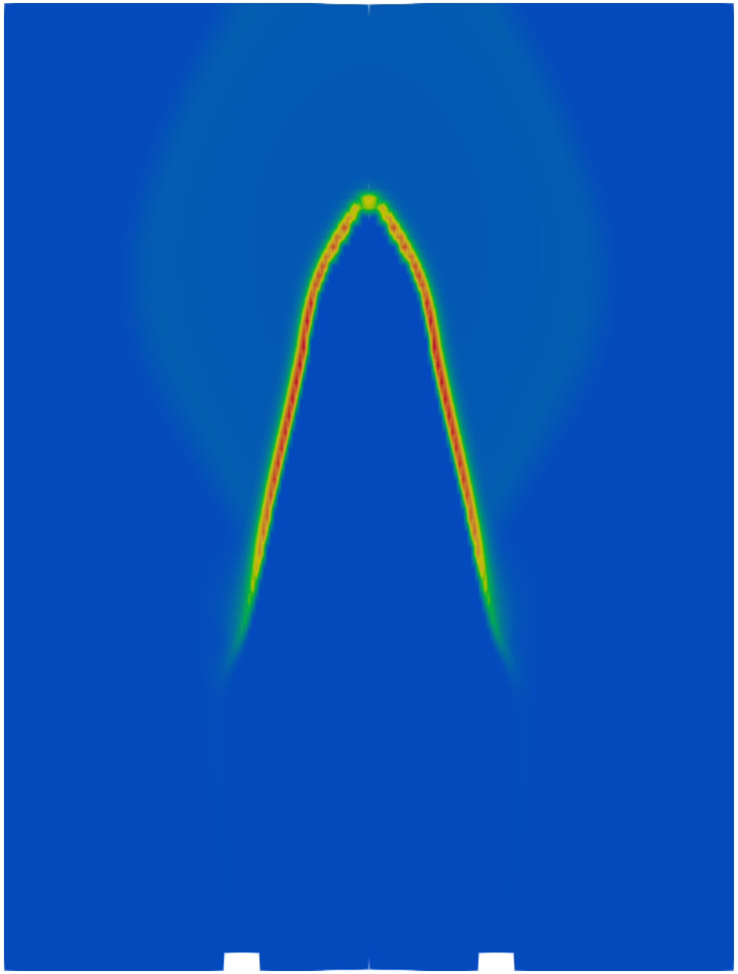


Progress variable reaction rate
@ t = 0.20s

Two dimensional flames

Results





Progress variable reaction rate
@ t = 0.46s

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

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

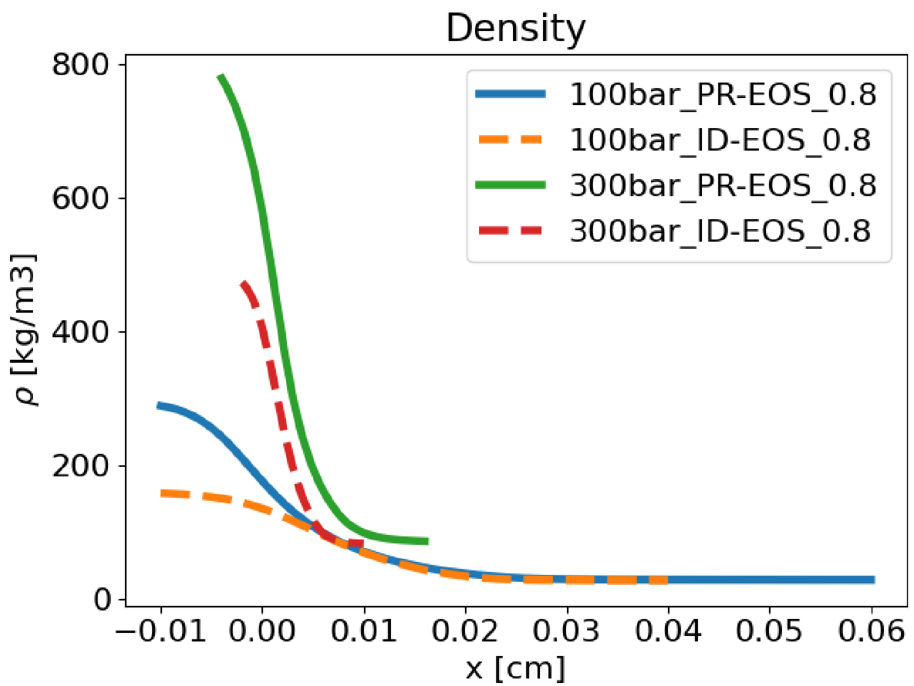
Thank you for your attention.

Federico Lo Presti

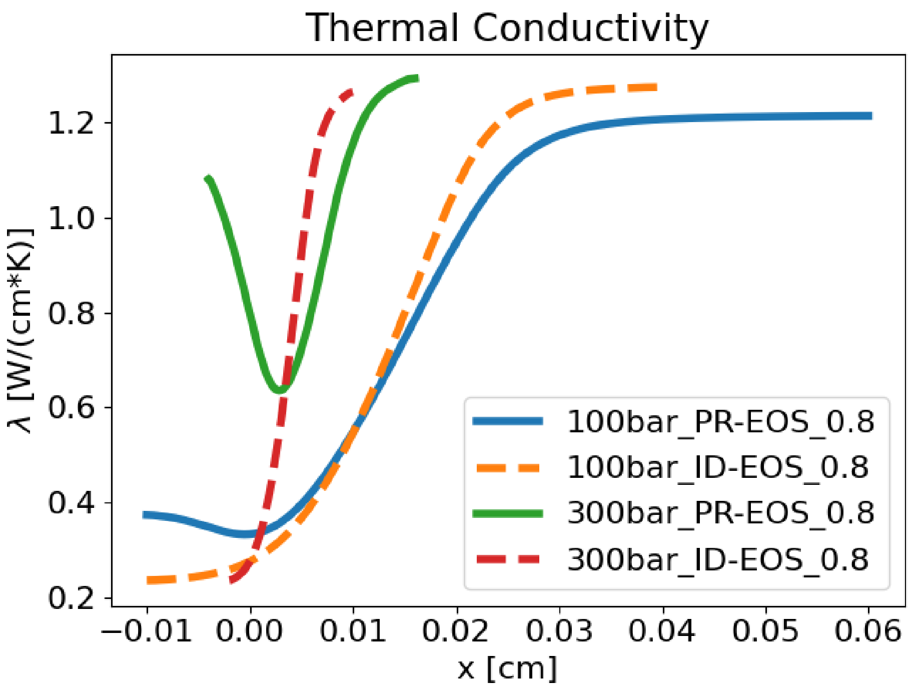
federico.lopresti@rub.de

One dimensional flames

OxyFuel combustion



$X_{CO2} = 0.8$



$X_{CO2} = 0.8$

One dimensional flames

OxyFuel combustion