# RUB

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

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**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
- <u>Carbon Capture and Sequestration</u>
  g. in directly fired supercritical CO<sub>2</sub> power cycles
   oxyfuel: no NO<sub>x</sub>
   higher density: lower size



## **Introduction and motivation**

#### Non-premixed

**Premixed** 





# Outline

- Introduction and Motivation
- One dimensional flames:
  - ° Chemistry solver
  - ° Chemistry mechanisms
  - $^{\circ}\,$  Equation of state, thermodynamics and transport
- Two dimensional application
  - ° Coupling CFD and chemistry solver
  - Bunsen flames results
- Conclusions and outlook



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**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

RUE

#### **Biogas mixtures**

	Fuel		Oxidizer		
Φ	$\mathrm{CH}_4$	$CO_2$	$N_2$	$O_2$	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

#### Validation at low pressure

#### Unburnt mixture T=300K



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#### Unburnt mixture T=300K





#### 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)





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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





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#### **OxyFuel combustion**

	Fuel	Oxidi	zer
Φ	CH <sub>4</sub>	CO <sub>2</sub>	<b>O</b> <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
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#### Unburnt mixture T=300K



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#### Unburnt mixture T=300K



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#### **OxyFuel** combustion



#### OxyFuel combustion



## OxyFuel combustion





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## **Two dimensional flames**

#### Coupling CFD solver with chemistry tables



- OpenFOAM + CHEM1D tables
- Unconfined Bunsen configuration
- Fuel: CH<sub>4</sub>, Oxidizer: 80% CO<sub>2</sub>, 20% O<sub>2</sub>
- 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 <sub>L</sub> )
200 bar	1.2691 mm/s	5.0764 mm/s (4 s <sub>L</sub> )
300 bar	1.5988 mm/s	6.3925 mm/s (4 s <sub>L</sub> )



# **Two dimensional flames**

#### Results

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



# Pressure Unburnt Mixture Velocity 300 bar $3.1976 \text{ mm/s} (2 \text{ s}_L)$ 300 bar $6.3925 \text{ mm/s} (4 \text{ s}_L)$ 300 bar $9.5928 \text{ mm/s} (6 \text{ s}_L)$ 300 bar $12.7904 \text{ mm/s} (8 \text{ s}_L)$ 300 bar $19.1856 \text{ mm/s} (12 \text{ s}_L)$







Progress variable reaction rate @ t = 0.15s





Progress variable reaction rate @ t = 0.20s





Progress variable reaction rate @ t = 0.46s



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# **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.

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#### OxyFuel combustion



#### **OxyFuel combustion**

