

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 Presti¹, P. Post¹, F. di Mare¹, J. van Oijen²

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



Some research trends in gas turbines:

- Hydrogen combustion
- <u>Carbon Capture and Sequestration</u>
 g. in directly fired supercritical CO₂ power cycles
 oxyfuel: no NO_x
 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

CHEM1D¹

- 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

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

RUE

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

Validation at low pressure

Unburnt mixture T=300K



Biogas mixtures

	Fuel		Oxidizer		
Φ	CH_4	CO_2	\mathbf{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





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)





Chemistry mechanism

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- AramcoMech2.0 reduced (37 species and 223 reactions)





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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OxyFuel combustion

	Fuel	Oxidi	zer
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



OxyFuel combustion

	Fuel	Oxidi	izer
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



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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: CH₄, Oxidizer: 80% CO₂, 20% O₂
- 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)		



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.

Federico Lo Presti

federico.lopresti@rub.de



OxyFuel combustion



OxyFuel combustion

