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

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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 CO₂ power cycles
- $\left\{ \begin{array}{l} \bullet \text{ reduce CO}_2 \text{ emissions} \\ \bullet \text{ oxyfuel: no NO}_x \\ \bullet \text{ higher density: lower size} \end{array} \right.$

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

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One dimensional flames

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>

One dimensional flames

Biogas mixtures

Φ	Fuel		Oxidizer		
	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

Φ	Fuel		Oxidizer		
	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)

One dimensional flames

Chemistry mechanism

- GRI 3.0 (53 species and 255 reactions, not validated for high p)
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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

- ID: Ideal Gas EOS, Nasa Polynomials, Power Law
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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 $T=300\text{K}$

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

One dimensional flames

OxyFuel combustion

One dimensional flames

OxyFuel combustion

One dimensional flames

OxyFuel combustion

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Two dimensional flames

Coupling CFD solver with chemistry tables

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
- $\text{Re} = 47 - 206$

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

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

Two dimensional flames

Results

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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One dimensional flames

OxyFuel combustion

One dimensional flames

OxyFuel combustion