Modeling and reduction of the LOx-Methane chemical kinetics for rocket engines applications

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Context

- Development of PROMETHEUS rocket engine in Europe for ArianeNEXT launcher [1]

➢ **Methane (CH_4) / Oxygen (O_2)** propellant

➢ Reduced costs

➢ Reusable engine

But high pressure and temperature combustion of CH_4/O_2 mixture not well understood …

[1] P. Simontacchi *et al.*, "Prometheus: Precursor of new low-cost rocket engine family," *Proc. Int. Astronaut. Congr. IAC*, vol. 2018-October, no. 1, pp. 1–12, 2018

THESIS TARGET:
develop CH_4/O_2 combustion model valid for rocket engines operative conditons

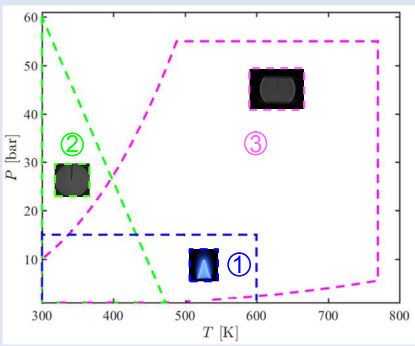
Model needs to be:

1) Consistent with experimental data (flame speed S_u)
2) Compatible with CFD simulation codes (model size)

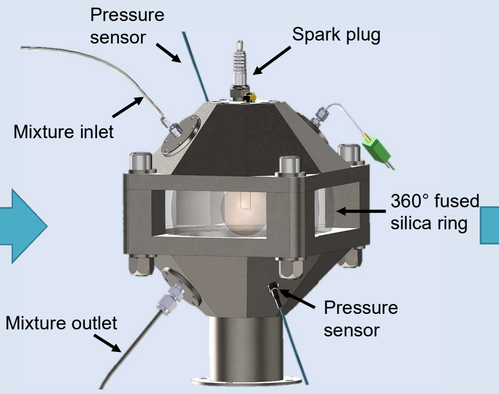
1. Experimental data acquisition

Measuring flame speeds at high pressure and temperature: **ISOCHORIC COMBUSTION**

1: Bunsen burner
2: Constant pressure chamber
3: Constant volume chamber



OPTIPRIME combustion chamber [2]

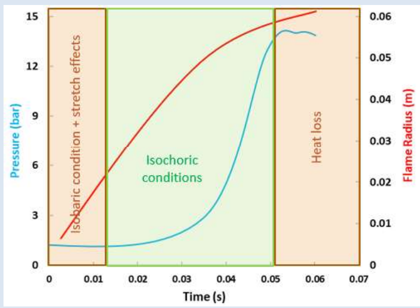


[2] F. Halter *et al.*, "Development of an optically accessible apparatus to characterize the evolution of spherically expanding flames under constant volume conditions," *Combust. Flame*, vol. 212, pp. 165–176, 2020,

Flame speed S_u computation

$$S_u = \frac{dR_f}{dt} - \frac{R_c^3 - R_f^3}{3\gamma_u R_f^2 P}\frac{dP}{dt}$$

Flame speed in the lab frame — Fresh gases expansion speed



2. Numerical modelisation

Experimental data vs chemical schemes
(numerical models)

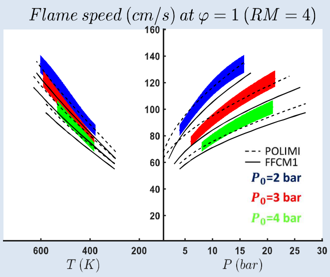
- Different mixtures tested:

➢ CH_4/air
➢ CH_4/O_2/Diluent $(He+Ar)$
➢ Pure CH_4/O_2

- Selected models:

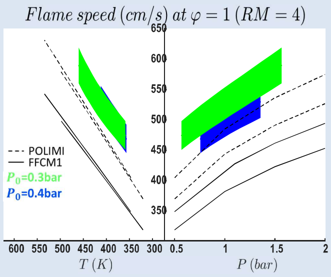
	FFCM-1 [3]	POLIMI C1-C3 [4]
Species nbr	38	114
Reactions nbr	291	1999

CH_4/O_2/Diluent (*He* +*Ar*)



→ POLIMI model consistent with experimental data in diluted conditions

Pure CH_4/O_2

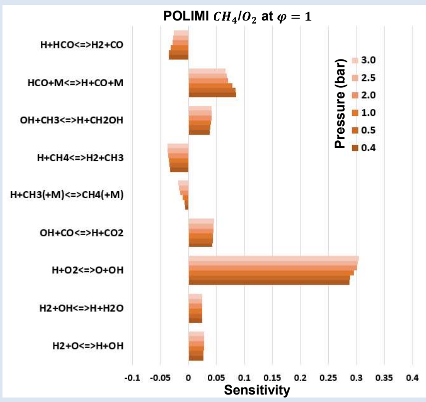


→ POLIMI model underestimate experimental data for pure CH_4/O_2 mixtures

Chemical schemes analysis and optimization
(numerical models)

Sensitivity analysis is required to understand and correct the discrepancies

Sensitivity on flame speed: $S = \frac{\Delta S_u}{S_u} / \frac{\Delta k}{k}$ with Arrhenius law $k = AT^b e^{-\frac{Ea}{RT}}$



- **Key reactions** are identified
- Their **reaction rates** can be modified (to a certain extent) to fit the experimental data. 2 methods currently tested:

➢ **Manual k optimization**
➢ **Arrhenius parameters global optimization** (via numerical code)

[3] "G.P. Smith, Y. Tao, and H. Wang, Foundational Fuel Chemistry Model Version 1.0 (FFCM-1), http://nanoenergy.stanford.edu/ffcm1, 2016."
[4] G. Bagheri, E. Ranzi, M. Pelucchi, A. Parente, A. Frassoldati, and T. Faravelli, "Comprehensive kinetic study of combustion technologies for low environmental impact: MILD and OXY-fuel combustion of methane," *Combust. Flame*, vol. 212, no. x, pp. 142–155, 2020,

Conclusion and perspectives

✓ Flame speed experimental acquisition for pure CH_4/O_2 in never before tested conditions
✓ Key reactions piloting S_u for different mixtures conditions identified. Different optimization methods currently tested
→ Reduction of the optimized scheme (code already tested on other cases) and implementation into CFD solvers for test cases calculations