Mechanical Engineering Summer Research Program 2021

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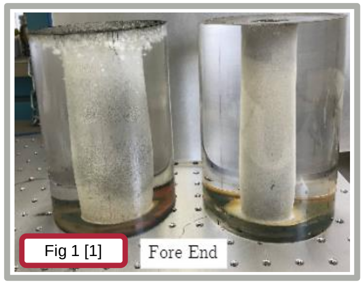
Reduced Kinetic Model for Hybrid Rocket Combustion Studies of MMA/GO_X

Introduction

Poly methyl methacrylate (PMMA) is a synthetic polymer used as solid fuel grain (Fig. 1) for hybrid rocket motors (Fig. 2) . In order to predict its combustion characteristics (burning rate, temperature, heat flux, etc.) in CFD simulations, it is essential to develop an accurate, compact chemical kinetic model for the oxidation of its primary decomposition product, MMA, as opposed to a computationally costly detailed model involving thousands of reaction and hundreds of species. Model reduction maintains important major species and intermediates to avoid losing performance accuracy.



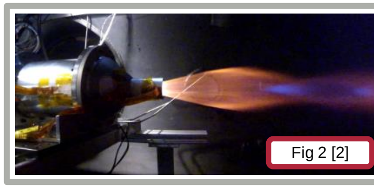


Fig. 1 – PMMA Fuel Grain after testing at ambient and low external pressure [1]

Fig. 2 – Hybrid Motor test in internal-vacuum chamber [2]

$$C_5O_2H_8 + 6O_2 \rightarrow 5CO_2 + 4H_2O$$

MMA + Oxidizer | Combustion Products

Objectives

This research entailed the analysis and validation of data from two MMA mechanisms against a detailed model and each other:

"Long" MMA Mechanism [3]	88 species, 1084 reactions
"Short" MMA Mechanism [4]	50 species, 320 reactions

- Conduct separate simulations of a premixed MMA/Air flat flame for each mechanism
- Compare measured burning velocities, mass/mole fraction results between reduced models and overall test run times
- Percent difference and points of agreement between mechanisms and detailed model results?

Burning Vel vs Equiv. Ratio Run Times (Fig. 3)

"Long" Mech [3]	*hh/mm/ss* | 01:40:03
"Short" Mech [4]	*hh/mm/ss* | 00:30:24

Materials & Methods

- Cantera module via Python (https://cantera.org/)
  - Gas solution object's unburnt temp (298K – 358K) and atm. pressure is set with premixed gas composition
  - Free Flame object created and solved, simulating freely-propagating flat flame
  - Equivalence ratios (Φ) span from lean to rich (0.7 - 1.3)
- Matplotlib for Python plotting (https://matplotlib.org/)

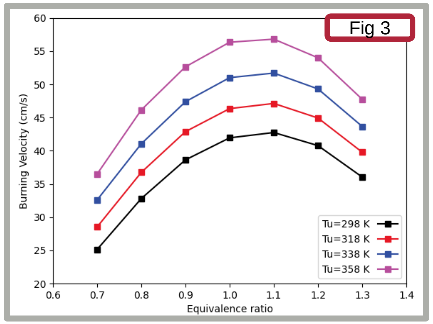
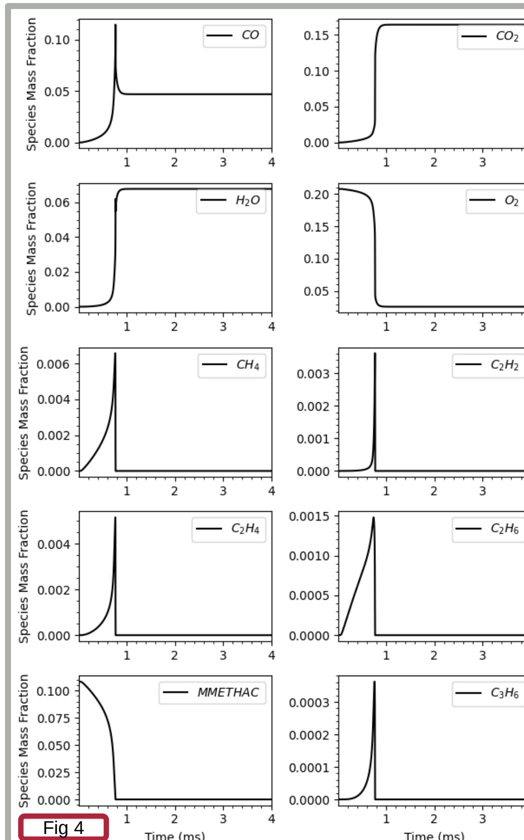


Fig. 3 – Laminar Burning velocity vs. Equivalence Ratio for "Short" Mechanism [4] ran with MMA/Air mixture at 298 K to 358 K and from Φ = 0.7 - 1.3

$$\phi = \frac{\text{fuel-to-oxidizer ratio}}{(\text{fuel-to-oxidizer ratio})_{\text{st}}} = \frac{m_{\text{fuel}}/m_{\text{ox}}}{(m_{\text{fuel}}/m_{\text{ox}})_{\text{st}}} = \frac{n_{\text{fuel}}/n_{\text{ox}}}{(n_{\text{fuel}}/n_{\text{ox}})_{\text{st}}}$$

Fig. 4 – Species Mass Fraction vs Time (ms) for "Long" Mechanism [3] ran with MMA/Air mixture at T = 1100 K, P = 1 atm, and Φ = 1.0



Results

- Run time dropped by factor of ~3 after model reduced from "Long" to "Short"
- After reduction, plots show 0.41% difference in Burning Vel. output averaged from 298 K to 358 K between mechanisms; max 0.64% difference at Φ = 0.7 and minimum 0.07% difference at Φ = 1.2
- "Long" Mech Mass Fraction profiles for fuel (MMETHAC), oxidizer (O_2), and major combustion products are consistent with publication's detailed/skeletal mechanism
- Smaller discrepancies seen for minor species mass fraction peaks (CH_4, C_2H_2, C_2H_6, C_3H_6)

Conclusion

The most recent reduced "Short" MMA Mechanism satisfactorily predicts major species profiles and laminar burning velocities over range of Φ at atmospheric pressure.

1) E. T. Jens, Ashley C Karp, Kyle T Williams et al.(Aug 2019) AIAA

2) E. T. Jens, et al.(2019) IEEE Aerospace Conference

3) S. Dakshnamurthy, et al (2018), Combustion Science & Technology

4) S. Dakshnamurthy, et al (2019) Combustion Institute