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Abstract #XXX (to be filled by the organizers)

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### Title

## Analysis of Detailed-Chemistry Schemes for the Numerical Simulation of Supercritical LO<sub>x</sub>/CH<sub>4</sub> Flames

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### Abstract

The increasing interest in reusable LO<sub>x</sub>/CH<sub>4</sub> first-stage liquid rocket engines requires the further development of suitable computational fluid dynamics tools for the reliable design and analysis of such engines. Shifting from classical LO<sub>x</sub>/H<sub>2</sub> to methane as a fuel involves many challenges for the accurate modelling of chemical effects as the characteristic time scale for LO<sub>x</sub>/CH<sub>4</sub> is significantly longer than for hydrogen. This can result in, for example, flame lift-off and reattachment effects that may cause substantial combustion instabilities. Also, the injector wall temperature may play a more significant role than in classical LO<sub>x</sub>/H<sub>2</sub> engines. The purpose of this study is to compare numerical simulation results using a complex detailed-chemistry scheme with previous results obtained with a real-gas flamelet model. Additionally, a novel machine-learning based approach for the efficient tabulation of chemical reactions rates will be tested and compared against results with the full reaction mechanism.

This comparison will be based on two dedicated numerical testcases which have been used extensively in the past: The first one is a modified version of the real-gas 2D mixing test case of Ruiz et al. [1]. This computationally cheap setup allows for a detailed study of mixing and chemical reactions under thermodynamic conditions that are representative for rocket engine. A more realistic setup will be investigated with the second test case HF-10 from the Franco-German Rocket Engine Stability Initiative (REST). In this test case, the flame behind a realistic single shear-coaxial injector will be investigated in a 3D simulation at supercritical conditions. This paper continues our work on the HF-10 test case [2,3] presented at the EUCASS 2022 conference and allows for a more general assessment of chemical non-equilibrium effects at supercritical pressures commonly encountered in liquid rocket engines.

### References

[1] Ruiz, Anthony M. and Lacaze, Guilhem and Oefelein, Joseph C. and Mari, Raphael and Cuenot, Benedicte and Selle, Laurent and Poinso, Thierry (2016). *Numerical benchmark for high-Reynolds-number supercritical flows with large density gradients*. AIAA Journal 54.5, 1445-1460.

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