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REDUCED KINETIC MECHANISMS FOR METHANE-OXYGEN ROCKETS TO MARS

Abstract

The use of methane as a rocket fuel has received increased attention recently for numerous reasons; 1) availability as a low cost fuel on Earth, 2) it is non-toxic and easier to handle and store then most rocket fuels, and 3) its availability elsewhere in the Solar System for in situ resource utilization (ISRU). As humans look to establish permanent outposts and eventually colonies beyond Earth, such as on the Moon and Mars, liquid methane is an attractive fuel. On Mars methane can be produced from carbon dioxide and hydrogen, which are available on Mars, using the Sabatier process. Saturn's moon Titan has large amounts of methane on the surface and in the atmosphere. To develop and optimize a Liquid Methane-Liquid Oxygen (LM-LOX) rocket combustor required detailed 3-D Computational Fluid Dynamics (CFD) using a real gas equation of state and a chemical kinetic mechanism valid for the fuel and operating conditions. To keep computer runtimes tractable a reduced kinetic mechanism is normally used. A full mechanism would have on the order of 32 species for methane combustion without nitrogen chemistry. While a reduced mechanism ideally would have 10-12 species to keep the computer runtime and memory requirements reasonable. A common method to reduce a kinetic mechanism is using comparing laminar flame speeds, counter flow flames and transient Perfectly Stirred Reactors (PSR's) profiles. A problem with these methods is they don't account for the effects of small scale turbulence on the reaction rates. A new tool that does account for this effect is the Conditional Moment Closure (CMC) method. Here the scalar dissipation (also called micro-mixing) directly accounts for the interaction of the small scale turbulence on the chemical reactions. As the scalar dissipation is varied, the pathways the reactants take to products changes, highlighting which species and reaction rates are important at a given turbulence level. Here the CMC method is used to reduce the detailed GRI1.2 methane mechanism and show which species are important at different turbulence levels. The detailed mechanism is reduced one species at a time until the mechanism can no longer account for the effects of turbulence. This determines the minimum number of species required to accurately model the target flame and operating conditions. The improved reduced mechanism will provide higher fidelity modeling of liquid methane rocket combustion, in the quest to develop a manned rocket to Mars using ISRU fuel for the return trip.