IAF SPACE PROPULSION SYMPOSIUM (C4)
Solid and Hybrid Propulsion (2) (4)

Author: Mr. Vinicius Rossetto
Instituto Tecnológico de Aeronáutica (ITA), Brazil

Prof. Rene Gonçalves
Aeronautic Institute of Technology (ITA), Brazil
Prof.Dr. José Rocco
ITA-DCTA, Brazil

STUDY OF POTENTIAL USE OF MAGNESIUM/TEFLON/VITON PYROTECHNIC COMPOSITION AS AN IGNITOR FOR SOLID ROCKET MOTORS THROUGH COMPUTATIONAL SIMULATIONS USING MOLECULAR DYNAMICS (MD).

Abstract

A solid rocket motor ignitor is a device used to initiate the combustion of the solid propellant in the rocket motor. Typically, it consists of a pyrotechnic material or an electrically heated element that generates enough heat to ignite the propellant. The ignitor is placed in direct contact with the propellant or in a location where the heat it produces can effectively start the burning process. Once activated, either by electrical current or an external ignition source, the ignitor ignites the propellant, triggering the combustion process that powers the rocket. This study explores the potential use of Magnesium/Teflon/Viton Pyrotechnic Composition as an ignitor for solid rocket motors through computational simulations using molecular dynamics (MD). The focus is on modeling the molecular interactions and thermal decomposition of key compounds, such as ammonium perchlorate and metals, commonly found in decoy flares formulations. By simulating these interactions under extreme temperature and pressure conditions (up to 3000 K and 1000 atm), the research aims to assess the flare's ability to generate sufficient heat and thermal radiation to effectively ignite solid propellants in rocket motors applications. The simulations were performed using LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), a powerful tool for MD simulations, to examine the atomic-level behavior of the flare materials. LAMMPS enabled detailed modeling of the decomposition reactions, including bond-breaking and energy release mechanisms of the flare components. The results showed that under the specified conditions, the flare produced a peak thermal output of approximately 6 MW/m, sufficient to initiate combustion in a solid rocket motor. The study also investigated the optimization of the flare's composition by varying molecular configurations. These simulations indicated a 15