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DETERMINATION OF SOLID FUELS REGRESSION RATE BY REACTIVE MOLECULAR DYNAMICS SIMULATIONS

Abstract

Development and optimization of solid fuel formulations are usually time consuming and expensive. Computer simulations methods are usually the best alternative, but there are not many ab initio methodologies which can provide specific info (ballistic data) of new materials and/or systems. A methodology was developed for evaluating the regression rate of solid fuel grains using reactive molecular dynamics simulations. In this method, the solid grain is built using a moderate to large number of molecules, and the oxidizer flows through it. Combustion occurs by the contact between the propellant pair, and the fuel gets dragged into the flow. Through time, the grain thickness is evaluated, thus determining the regression rate. In this work, paraffin was used as the solid fuel (mono-perforated cylinder) and gaseous oxygen as the oxidizer. The oxidizer temperature was increased to enable the ignition and combustion of the system. Although the complete combustion is not reached before leaving the "combustion chamber", the obtained regression rate was approximately 0.9 mm/s, in accordance with experimental data found in the literature. This method can become one of the best tools in developing propellant formulations due to the accuracy and speed.