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MODELING THE FRONT PROPAGATION OF THE THERMITE REACTION BETWEEN HEMATITE AND ALUMINA WITH NON-CONSTANT THERMODYNAMIC PROPERTIES

Abstract

Thermite reaction is a self-propagating highly exothermic reaction which requires low energy consumption and can react in oxygen-free environments. Since energy and oxygen in space is limited, there have been studies of applying thermite in space welding, and combustion-based production of materials from lunar regolith. Moreover, it has some other aerospace applications, such as to ignite rocket motors, to increase the combustion performance of solid-propellant rockets as additive in propellants, and to produce thrust for underwater propulsion. However, the physicochemical mechanisms that govern a thermite reaction are not yet completely understood. Despite being generally treated as an overall basic condensed-phase reaction, it is a process with high complexity due to all the physical and chemical events included, such as phase changes, decomposition, surface tension, droplet collisions, and others that make a difficult task to foresee and model a thermite reaction. Consequently, there has been few works in modeling this process, which induced the present study in modeling the common hematite-alumina reaction, solving the equations of mass and energy conservation by applying a five-points finite difference method. The analysis is transient in order to observe the reaction front moving along a one-dimension radial space, and the consumption of reactants, aiming to match the temperature and progression rates achieved experimentally in literature. Although the present model attempt to simplify the problem in order to enable the numerical study, there was some care about approaching the numerical results to experimental ones. Therefore, whenever possible, it was considered some complex mechanisms such as phase changes, heat losses, and the thermodynamic properties dependency on temperature and species concentration. At the end, a good approach between the present numerical results and experimental results from literature was observed.