The Study of Computational Chemistry Simulation of Ferrocene for Solid Propellant

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***Abstract*—Ferrocene $(Fe(C_5H_5)_2)$ is an organometallic compound which its structure consists of two cyclopentadienyl (C_p) rings bound on opposite sides of a central metal atom. This compound is usually added into rocket's solid propellant as a burning rate catalyst. However, this composition always migrates from the propellant system by both diffusion and surface migration mechanism that causes the unpredictability of the burning rate which in turn renders unpredictable rocket performance Therefore, the study of the method to investigate the role of Ferrocene in biological systems is highly significant. This paper proposes the use of molecular simulation to study the properties of Ferrocene molecular systems to get a deeper understanding of the physics of electronic correlation in real materials. The result from the studies shows that Gaussian and Monte Carlo is the suitable method to simulate the role of Ferrocene in biological systems.**

I. Introduction

A propulsion exploration is in fact one of great significance to the aerospace industrial development. Basically, a propellant is the most important ingredients to provide a driving force for rockets to hit the target. The high efficiency properties of solid propellant are the burning rate stabilities and a low pressure exponent. To achieve this goal, the best method is to add a burning rate catalyst into the compound. Currently, the burning rate catalysts mainly include transition metal oxides, nano-metal particles, metal chelates, Fc-based polymers and derivatives. Ferrocence (Fc-based) is an organometallic compound that the structure consists of two cyclopentadienyl rings bond on opposite sides of a metal atom. Their derivatives are commonly used as ligands for transition-metal catalyzed reactions. This compound is usually added into solid propellant as a burning rate catalyst. Because of its small size molecule, this composition always migrates from the propellant system by both diffusion and surface migration mechanism. As a result, the migration further destroys propellant homogeneity and permits higher burning rates only on the surface of the propellant than throughout the remainder of the propellant. This undesirable circumstance causes the unpredictability of the burning rate which in turn renders unpredictable rocket performance.

A. Solid Propellant

Solid propellant has several connotations, including the rubbery or plastic-like mixture of oxidizer, fuel, and other ingredients that have been processed and constitute the finished grain as in Fig. 1. The propellant is contained and stored directly in combustion chamber for a long time (5-20 years). The way that can determine propellant efficiency is to test and find the burning rate of the new propellant.

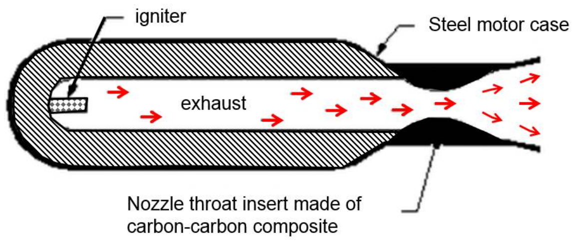

Fig. 1. Solid Propellant Rocket

B. Propellant ingredients

The propellant ingredients are categorized by major function, such as oxidizer, fuel, binder, plasticizer and curing agent. The ingredient properties and impurities influence on the propellant characteristics. A minor change in one compound can cause measurable change in ballistic properties, physical properties, migration, aging and manufacture.

C. Burning rate

The burning rate of solid rocket propellant is a function of propellant content which depends on type of propellant. The content of propellant mixtures directly affects the burning rate. Factors that can change the burning rate are as follows:

- Addition of catalyst materials or new burning rate enhancer [1], [2].
- Reduction of oxidizer particle size [3].
- Increase of the percentage of oxidizer agents.
- Increase of the amount of binder or oxidizer agent enhancing burning rate.
- Addition of metal rods or metal fibers into the fuel.

D. Migration problems

During development of a new or modified solid propellant, it is comprehensively or characterized. This includes the testing of the burning rate in many different ways, under different condition such as: temperatures, pressures, impurities, and conditions. Characterization also requires measurement of physical, chemical, manufacturing properties, ignitability,

978-1-4799-8168-7/15/$31.00