Analysis of a Pyrovalve Firing: Estimating Pyrotechnic Reactions

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The NASA White Sands Test Facility has developed a computational modeling technique that uses a thermodynamic equilibrium code to assist in evaluating experimental data taken in the harsh environments created by combusting pyrotechnics. One such environment ensues when a NASA standard initiator (NSI) is fired into a narrow aluminum channel as part of the pyrotechnic chain in a pyrovalve.

To ensure pyrovalve discharge, a redundant pyrotechnic chain featuring two NSIs in parallel with a booster charge may be used. A common configuration takes the form of a "Y," where the fiery output from each NSI is directed through channels that lead to a chamber at the base of the "Y" into which a booster pyrotechnic charge is attached (figure 1). The pyrovalve design uses a Y-shaped primer chamber assembly, usually referred to as a Y-PCA. The booster, when ignited, generates gas that drives the cutting ram of the pyrovalve. Different firing sequences may be used so that one or both of the NSIs are ignited.

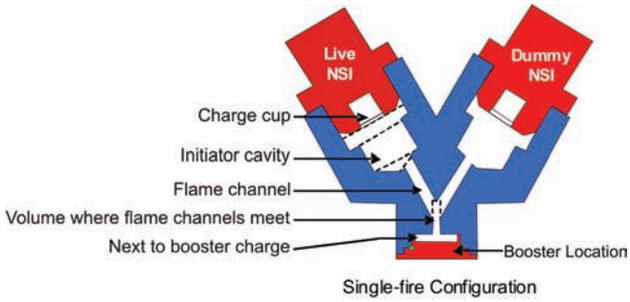

Fig. 1. *Cross section of the Y-PCA pyrovalve showing the various volumes.*

Study of system performance shows that the time to ignition of the booster is variable, the types and amounts of energies needed to ignite the booster propellant are not well understood, and it is unclear what system variables are responsible. In some instances, initiation of a single NSI has inadvertently caused the firing of the second NSI. We analyzed a pyrovalve firing to identify thermal and chemical processes leading to booster ignition to better understand this energy transfer process. Basic questions driving the investigation revolved around whether the booster propellant was directly ignited by penetration of driven materials or heated above the autoignition temperature. Physical observations, posttest metallurgical analyses, and in-situ temperature measurements were difficult to interpret. However, recessed pressure gauges showed reliable time-dependent behavior.

To develop an understanding of temperature behavior in the pyrovalve environment, we applied the notion that if the state of the pyrotechnic reaction products could be computed, knowledge of two state variables could allow determination of other state variables. The system of the reaction products is distinguished as separate from the fixture and booster, the environment into which energy from the reaction is lost. Pressure is the state variable that is measured; for each time a measurement is captured, the state of the reaction products, including the enthalpy, can be evaluated. The total energy of the pyrotechnic propellant and the volume into which it burns, or energy density, are also known at the start. From measurement to measurement, the loss of energy to the "environment" can be noted. For each new state, a temperature can be computed. We achieved this approach by using the NASA-developed chemical equilibrium with applications, a thermodynamic equilibrium code, and by keeping track of the energy lost to the environment.

Chemical equilibrium with applications calculations applied to propellant combustion

Combustion products interact with the cavity's internal surface. The reaction products partially pressurize the initiator cavity and rapidly flow through the flame channel to the booster cavity. This flow pressurizes the remainder of the Y-PCA. Depending on the test configuration (single- or dual-fire) and the amount of propellant, pressurization reaches different levels at different times. During the pressurization period, heat is also conducted to the surroundings. The release of energy by the chemical reaction occurs very rapidly: 10 to 20 µs (short compared to the 1 to 4 ms to heat and pressurize the entire Y-PCA system).

The amount of zirconium potassium perchlorate (ZPP) combusted for a specified Y-PCA volume represents a confined system that has a constant, common pair: internal energy and specific volume (density). This in turn determines the other states (e.g., temperature and

pressure) to maintain equilibrium. We subsequently used the parametric determinations of temperature and pressure to convert pressure-time states to temperature-time states. The chemical equilibrium with applications code does not account for energy losses; but in this analysis, the difference between code determinations of different states can be considered a measure of energy loss.

We performed chemical equilibrium with applications computations stipulating temperature-specific volume for the energy density in question and over a wide range of temperatures. Pressure-temperature state relationships for energy densities represent key charge loads (figure 2). Based on these data, we performed internal energy-specific volume calculations to determine the maximum pressure and temperature.

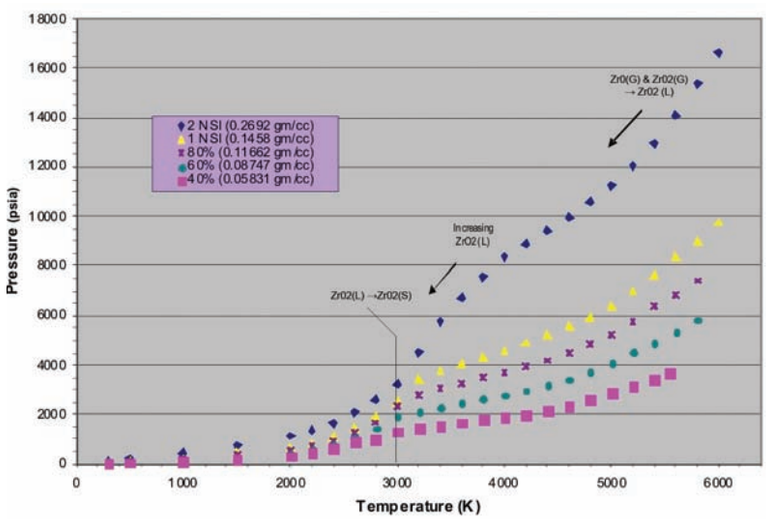

Fig. 2. *Pressure–temperature state curve.*

For a simple ideal gas, the relationship between pressure and temperature is linear. ZPP combustion creates a multicomponent hot gas and vapor at high pressure; within specific temperature ranges, the overall relationship is very roughly linear. Examination of product species predicted by chemical equilibrium with applications showed that several phase transitions and chemical reactions appear to contribute to the shifts in slope. Pressure-time data can be transformed using the pressure-temperature state relationship to develop a temperature-time relationship.

The pressure-temperature state curve shape is influenced by chemical recombination and phase-change processes occurring within the multicomponent mixture. At the elevated temperature of the reaction, the chemical equilibrium with applications code predicted more than 40 species in equilibrium, many of which are compounds related to the constituents of Viton®-B, a relatively minor constituent by weight. The primary species are related to the fuel, the oxidizer, and their combustion products.

System state determined by pressure vs. time data

Each unique pressure, as determined by the pressure-time data and combined with knowledge of the initial energy of the system, gives the state of the system, including losses to outside the system. For any given pressure, a corresponding temperature and amount of heat loss can be found to maintain equilibrium. We used the pressure-temperature state curve for a given energy density to transform selected points on the pressure-time curves to give a temperature-time curve. These curves are plotted in figure 3 for tests representing energy densities of interest.

On the scale shown, initial combustion of ZPP occurs during the first 20 µs (a fraction of the first tic mark in figure 3). The range of times over which single- and dual-fire booster ignitions happen as well as the solidification temperature for zirconium oxide (ZrO_2) are drawn in for comparison purposes. Interpretation of temperature vs. time results is not covered in this report, but we did propose several ignition modes based on the information developed and the observed behavior for booster ignition.

Conclusions

Heat transfer between the hot reactants and the Y-PCA body is greatly influenced by the phase change of ZrO_2 from liquid to solid and by the chemical equilibrium with applications-predicted property that increased liquid ZrO_2 formation is favored by higher Y-PCA system pressures

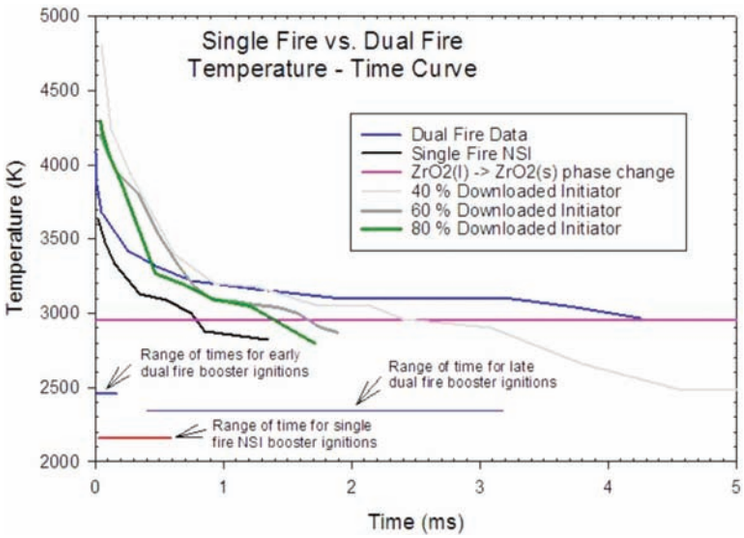

Fig. 3. *Temperature-time representations.*

at lower reaction system temperatures. As a consequence, for the range of charges examined (40%, 60%, and 80% downloaded, NSI, and dual-fire), the lower ZPP charge densities produce higher temperatures but less liquid ZrO_2. This contributes to the difference in heat transfer behavior between the single- and dual-fire events (two 100% NSIs) within the geometry of the Y-PCA fixture.

In the single-fire case, reaction products flow over the top of the booster cover into the unfired leg of the Y-PCA. The difference in flow for dual-fire events favors solidification of greater amounts of liquid ZrO_2 upstream. The liquid ZrO_2 transfers most of its heat content to whatever surface on which it solidifies. By contrast, the single-fire event, with only half the reactants, flows proportionally more reactants over the top of the booster, and more rapidly. Single-fire booster ignition events correlate with the period of greatest heat transfer.

Heat transfer in dual-fire events occurs more slowly as a "heat soak" process, probably driven by heat exchange of gaseous potassium chloride (KCl). Interpretation of chemical equilibrium with applications results suggests that KCl, the lighter reaction product that persists as a gas until it condenses (at much lower temperatures than the ZrO_2), is more effective than ZrO_2 at carrying energy to the booster at times when flow has stopped. The Y-PCA fixture requires reaction products to traverse the narrow flame channels, which join at a short channel (the leg of the "Y") before passing into the larger booster cavity. Hot KCl gas more readily penetrates through the channels. Posttest analysis of deposited reactants shows the presence of relatively more KCl in the booster region. This correlates with the later range of times for dual-fire booster ignition events.

The violent environment created when an NSI combusts inside a pyrovalve is difficult to characterize using experimental measurement techniques. This overview shows that by using the chemical equilibrium with applications as well as knowledge of ZPP reactants and physical volume and time-dependent pressure measurements, other state parameters for the reaction can be estimated. We determined computed values for reactant temperature vs. time, species, enthalpy, and internal energy.

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