3.2 Combustion and Energetic Materials

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Overview

Combustion of solid propellant composed of energetic materials is the driving thermomechanical force in the operation of a solid rocket motor. Accurate modeling and simulation of the combustion and resulting regression of solid propellants entails research activities in several areas, including the description and propagation of the propellant combustion interface, modeling of solid propellant flames, combustion instability analysis, and constitutive modeling of energetic materials.

The Combustion and Energetic Materials (CEM) group has a hierarchical strategy for developing solid propellant combustion models based on incremental physical/modeling complexity and parallel experimental validation. Under this strategy the daunting complexity of composite solid propellant combustion is attacked by isolating various physical/chemical phenomena within a lowest dimensional model necessary to address each level. Non-aluminized propellant issues are tackled first and then aluminum is added.

Radiative Properties of Burning Aluminum Droplets in Composite Solid Propellants (Harrison and Brewster)

Thermal radiation from burning aluminum droplets generated by combustion of aluminized solid propellants in propulsion systems (e.g., solid rocket motors) represents a potentially important and yet largely unknown heat transfer contribution in many areas of these systems, including internal insulator surfaces, nozzles, and the propellant surface. The purposes of this research are to develop a model of radiation emitted by burning aluminum droplets in solid propellants and to validate the model through experimental observations of emitted infrared intensity. During the past year a model for predicting emitted intensity from a burning aluminum droplet has been developed and experiments have been run over a range of pressures (1 to 40 atm) and wavelengths (3-5 µm).

The problem of thermal radiant emission from burning Al droplets is complicated by the fact that there is a very hot but optically thin, luminous alumina particle laden flame standing away from the Al...
droplet surface. There is the potential for substantial emission by this non-isothermal, optically non-homogeneous, reaction zone as well as by the Al droplet surface. Furthermore the system’s behavior could be quite different at different wavelengths; the behavior in the important infrared region could be quite different than that indicated by typical visible (optical/video) imaging, hence the need for infrared imaging and spectrally/spatially resolved modeling. The model developed accounts for non-gray emission by the hot, molten aluminum surface as well as non-gray emission by sub-micron, molten aluminum-oxide particles that populate the non-isothermal, detached, diffusion-flame envelope.

Typical experimental results for emitted intensity at 3.42 μm and 1 atm are shown in Figure 3.2.1. The thin rectangle at the center of the droplet image indicates the region from which the indicated intensity profile was taken. Intensity is seen to peak near the center of the droplet. In Figure 3.2.2, a comparison between modeled and experimental intensity is shown for these conditions. The intensity is plotted as the ratio of the burning aluminum droplet intensity to the intensity of a hot nichrome ribbon used for calibration. The model curve with the short dashed line (“model – with smoke envelope”) shows the prediction based on best guesses about optical and thermal properties of the aluminum droplet and the oxide-laden flame envelope region. Without adjustments the agreement is reasonable. For comparison, two limiting model predictions are also shown, one with the flame (smoke) envelope removed and one with the flame envelope made artificially optically thick. For optically thin smoke/flame conditions there is a predicted secondary maximum away from the center of the droplet at the location of the detached diffusion flame. No prominent intensity is observed experimentally, however, in this region. This is in contrast to video (primarily visible very near infrared) imaging. The results of model and experiment thus suggest that in the infrared region (unlike the visible region) the flame envelope emission contribution is negligible and the aluminum emission contribution dominates. Further experiments and modeling are being conducted to verify these findings and to explore the effects of pressure and other variables.

Aluminum Effects in Combustion of Composite Solid Propellants (Mullen and Brewster)

The effects of combustion of non-metalized oxidizer/fuel constituents Ammonium Perchlorate-Hydroxy-Terminated Polybutadiene (AP/HTPB) on aluminum agglomeration, ignition, and combustion in aluminized composite solid propellants are not well known. Neither are the effects of aluminum combustion on AP/HTPB behavior, although it has widely been thought that aluminum does not affect Al/HTPB combustion significantly since global (macroscopically averaged) burning rate does not seem much affected. Better understanding of the fundamental combustion of three-dimensional aluminized AP-composite solid propellants is needed and can be gained through investigating the behavior of aluminized laminate configurations. Laminate propellants allow for a more controlled study of the effects of AP/HTPB oxidizer-fuel components on the ignition, agglomeration, and combustion of aluminum as well as the inverse effects.
The two primary variables thought to affect aluminum agglomeration and ignition are the size or length-scale of the fuel-rich “pocket” between coarse AP particles and the pressure. Both of these variables are known to have a dominant influence in determining the AP/binder flame structure (i.e., whether the flame is split-diffusion or merged-premixed). The former (length scale) also influences the amount of aluminum in close spatial proximity available to agglomerate. Previous research in our group investigated AP/HTPB flame structure in non-aluminized laminate propellants and showed the effects of pressure and length scale (center fuel-layer thickness); Figure 3.2.3 shows a typical image (left) for conditions of 15 atm and 1000-µm fuel layer where the AP/HTPB flames are split and located near the AP/HTPB interfaces. As a result the fuel layer surface protrudes sharply upward. (At low pressures and small length-scales the flame structure tends toward merged-premixed.)

New results obtained during the past year with aluminized laminates has produced surprising results. Conventional models and understanding would suggest that addition of aluminum has little effect on AP/HTPB flame structure and burning surface structure. Recent results seem to indicate that at least part of that understanding may be incorrect. Figure 3.2.3 (right) shows an image with aluminum added. While the primary, coarse-AP/HTPB flame structure appears to still be split (diffusion), as evidenced by the location of Al droplet ignition, the fine-AP/HTPB surface profile is not protruding but flat. Thus laminate propellants show that simply adding Al has a profound affect on combustion of the fine-AP/HTPB flame zone over the fuel-rich zone. These observations provide data for further refinement of heterogeneous propellant combustion models and simulations of aluminized propellants.

Multiscale Modeling of Solid Rocket Motors: 2-D Quasi-steady Burning Using Parallel Multigrid Algorithm (Stewart and Bhattacharjee)

A multigrid acceleration technique with time integration is being implemented for the problem of efficiently computing the stable burn-back of a 2-D solid rocket motor when the motor is in the quasi-steady burning regime of operation. For large rockets such as the space shuttle solid rocket booster, the problem of quasi-steady solid rocket motor core flow is analogous to the steady aerodynamic flow past a large aircraft flying at speeds such that compressible flow effects must be included. The time integration strategies that have been developed for such applications are used to simulate solid rocket motor grain burning and to compute a series of realizations of steady flows as the grain burns back to near completion.
by a slow regression of the burning solid propellant. A straightforward two-timing, multiscale asymptotic analysis of the quasi-steady rocket burn developed in a previous paper will be used to advance the propellant interface from steady states with frozen geometry. Preliminary computations show speedups on a serial processor of 4 to 5 times that over a direct Euler solver for the same two axisymmetric geometry. Work is currently under way to implement the algorithm on parallel processors using domain decomposition. We anticipate speed ups that scale linearly with the number of processors, such that 256 processors (say) offers a possible speed up of 1000 times (at a fixed spatial resolution) to achieve a steady frozen configuration that is to be advanced by the surface regression algorithm (Figures 3.2.4 and 3.2.5).

Shock Initiation via Void Collapse (Parker and Austin)

The formation of local regions of energy release or hot spots is critical to detonation initiation in heterogeneous energetic materials. Hot spots are formed due to shock interaction with material heterogeneities, including voids in and between explosive crystals. We study the fundamental mechanisms of shock-void interaction relevant to condensed phase detonation initiation in a simplified system with dynamic, spatially resolved experimentation.

A layer of gelatinous material containing one or more voids is sandwiched between two optically accessible plates. A 152mm diameter aluminum bullet is accelerated by a gas gun and impacts the test mate-

Fig. 3.2.4: Instantaneous flowfields, for (from top down) Mach number, pressure, density, and x and y velocity components, for three different times computed with high order Euler solver, with resolution of (560 x 40).

Fig. 3.2.5: Steady state Euler solution for coarsest grid (140x10) and intermediate grid (280 x 20).
material, transmitting a shock wave with velocity 1850 m/s and post-shock pressure of 0.25Gpa (Figure 3.2.6). A high speed camera capable of 80 frames with a 1 microsecond interframe time is used to track the shock. The illumination for the experiment is provided by a 2w 514nm diode laser pulsed by passing the light through an acousto-optic modulator.

Initially, static compression testing was used to identify appropriate material properties and yielded encouraging results. Recently, high speed shadowgraph movies tracking the shock propagation through the gel have been made. The newly acquired diode laser has solved illumination problems that were limiting the resolution of the images.

Three-Dimensional Propellant Combustion Simulation (Buckmaster, Jackson, Massa, Wang)

The research group of Jackson, Buckmaster, Massa and Wang has been engaged for a number of years in the numerical simulation of three-dimensional heterogeneous solid propellant combustion. To this end we have, for the first time, created a three-dimensional code that fully couples the propellant solid physics with the gas-phase combustion in a non-planar non-steadily regressing propellant surface. We have validated burning rate predictions and the variations of these rates with propellant morphology by comparisons with experiment, without the use of curve fitting with three-dimensional results. We have, for the first time, been able to examine numerically the impact of acoustic waves on a burning heterogeneous propellant, and describe the properties of the reflected wave, a crucial issue in rocket chamber stability. Furthermore, we have, for the first time, been able to describe the proper injection boundary conditions for LES simulations, necessary for meaningful solid rocket motor simulations. For aluminized propellants we have developed algorithms that accurately predict the statistics of the aluminum agglomerates that form on the surface and which, after detachment, are of great concern to the rocket industry because of their impact on the nozzle. Aluminum agglomeration in the throat seriously degrades the specific impulse of the motor and significantly shortens the operational range of a motor. Hence this work has an enormous potential in that by tailoring the characteristics of the propellant packs to minimize aluminum agglomeration, one may be able to extend operating range of Air Force strategic missiles. A number of important projects have been worked on in the previous year, and are summarized below. These projects include the completion or modification of previous work, as well as the beginnings of new projects.

P1. **Rational Rocburn** We have developed what we call **Rational Rocburn**, a Rocburn module that is constructed by spatial averaging of **Rocfire**, accounting for unsteady effects on the propellant time scale. A key component of this module is a look-up table that properly accounts for the heat flux to the propellant surface from the **Rocfire** combustion field. This module has been incorporated into **Rocstar** and the central goal of the CEM group has now been achieved, albeit for non-aluminized propellants. Last year we published results for two-dimensional packs. We are currently extending the analysis to three-dimensional packs.

P2. **Rocpack** In order to simulate the combustion of three-dimensional composite propellants, a representation of the solid is required. To this end we previously developed **Rocpack**, a dynamic packing algorithm that takes as input industrial data size distributions, and generates a representative “virtual” solid propellant with the same volume fraction as that used in industry. The original version of the code only
packed AP particles, and was not user friendly. We therefore extended the code this past fiscal year to include a number of important features.

The particles can now be AP, HMX, RDX, aluminum, etc., or a combination, embedded in a binder, usually taken to be HTPB. The current version of the code is written in Fortran 90 and uses MPI. It has a user-friendly interface so that non-technical people can use the code. This new interface is called Rocprepack. Rocprepack and Rocpack are both in a CVS directory for others to download.

In the mixing process of real propellants, large AP particles are mixed first so that the binder coats each AP particle; smaller AP particles are then poured into this mixture. This generates a pack where the binder separates the large AP particles. To better simulate this process, we have added a “coating” parameter to Rocpack, which allows the user to define an averaged separation distance for all particles. A typical coating value might be 190 nm.

Typical packs range in size from as few as 30,000 particles, which can be generated on 16-processors in about one day, up to 500,000 particles, which requires 100-processors and takes approximately 36 wall clock hours to generate. Both ATK and Aerojet West have expressed interest in using this code in their Air Force sponsored research, and it is our intent to license the code to them. In the coming fiscal year we plan to make Rocprepack a GUI driven interface.

In addition to the modifications listed above, the inclusion of non-spherical particles, in particular ellipsoids, was added as a new feature. The capability to model non-spherical particles was added to study the effect of particle shape on burn rates. Combustion results using Rocfire show that if the ellipsoids are randomly oriented, then the average burn rate differs little from their spherical counterparts. However, if the ellipsoids are aligned in some preferred direction, then the average burn rate can be changed significantly. This might have practical implications in motor design, but we plan no further modifications unless asked by the rocket industry.

Finally, we are looking into extending Rocpack to include arbitrary shapes. We recently added the capability of packing rectangles, necessary as a first step in simulation igniters. More general shapes will be added in the coming year.

P3. Rocfire – Non-aluminized Once the “virtual” propellants have been built, they need to be “virtually burned”. To this end we have previously developed Rocfire; in the gas phase this solves the three-dimensional zero Mach number equations for a reacting gas, and in the solid phase solves the three-dimensional unsteady heat equation. The solid and gas are closely coupled using appropriate jump conditions and pyrolysis laws across their interface, which is represented using level sets, hereby allowing the surface to take on any shape the physics dictates. The code is written in Fortran 90 and uses MPI, and uses GMRES to speed up the pressure solver. Typical grid sizes are approximately 1-10 microns, while the packs are on the size of 1-2 millimeters. A typical output of Rocfire is shown in Figure 3.2.8. Our experience is that this size is sufficient for purposes of gathering statistics. To get the necessary statistics,
typical run time is approximately 2-3 days using 100 processors for a fixed pressure. To get a complete pressure history, the code needs to run for several weeks given dedicated computer time. A variation of \textit{Rocfire} (non-aluminized) has been developed using a three-step kinetics model rather than a two-step model as in the first implementation. Superior agreement with experimental burning rates of various Miller packs is achieved and further improvement in this respect cannot be expected. The new model leads to intrinsic instabilities under some circumstances, the stability boundaries of which cannot be expected to match reality, but there might be no resolution of this difficulty within the framework of global kinetics. We hope to revisit this difficulty in the coming fiscal year using the newly developed code \textit{Rocfit}, as described below.

P4. Acoustics \textit{Rocfire} has been applied to an important physical problem, namely the burning response to an impinging acoustic wave. There are serious rocket stability issues should the reflected wave have a larger amplitude than the incident wave. We have been able to compare the mass-flux response function and the velocity response function (both functions of frequency) and have shown to what extent they differ. Since the velocity response cannot be measure experimentally, whereas the mass-flux response can, it is always assumed that they are equal in making stability predictions, and we have described the errors that can arise in doing this. The original work was for two-dimensional packs, but we hope to revisit the problem in three-dimensions within the coming fiscal year.

P5. \textit{Rocfit} The use of detailed kinetic schemes is still too computationally intensive for three-dimensional simulations so global kinetic schemes are employed instead. However, global kinetic schemes involve a number of parameters that must be chosen in a rational way. To this end we have recently developed \textit{Rocfit}, a numerical software tool that uses a numerical optimization scheme based on genetic algorithms to choose optimal parameters. \textit{Rocfit} runs on an MPI platform using 100-processors, and takes about 12 hours to generate a set of parameters. \textit{Rocfit} is currently being used to calibrate the global kinetic parameters for HMX/HTPB propellants for which extensive experimental data are available. Figure 3.2.9 shows an instantaneous surface temperature profile for one HMX propellant pack. In the near future we will use \textit{Rocfit} to re-calibrate the AP/HTPB kinetic parameters, and compare burn rate results with previous work. It is expected that by using \textit{Rocfit}, the intrinsic instability mentioned earlier when using hand optimization, can be avoided.

P6. Far-field Solutions The CSAR code \textit{Rocstar} accommodates turbulence using large-eddy simulations. Here a new challenge, not present in traditional scenarios, is a proper accounting of the nature of the injected flow at the chamber/propellant boundary. Particularly for heterogeneous propellants, this flow and the vorticity it carries is neither steady nor spatially uniform. These fluctuations could well have an effect on the overall chamber flow and, indeed, there is a significant amount of experimental and computational work that demonstrates the effect of perturbations of initial or boundary conditions on the long-time or far-field solution of turbulent flow-fields. Of particular interest in rocket flows is the interaction between the omnipresent acoustic waves and fluctua-
ions of the injected flow, and a number of studies have shown how important this can be for certain parameter values. For these reasons alone, notwithstanding the significance of any findings, it is of interest to describe the nature of the flow-field at an intermediate distance above the propellant surface, intermediate in the sense that the distance is large compared to the scale of the flame structure, but small compared to appropriately defined flow scales. To this end the far-field of Rocfire (~ 1mm from the surface) is currently being examined for very large packs in an attempt to characterize the flow field fluctuations that should be used as boundary conditions for the LES simulations of the Fluids Group. Preliminary work has been carried out and implemented into Rocstar.

Figure 3.2.10 shows the most recent work. The combustion field beyond the flame zone has large velocity and temperature fluctuations (Figure 3.2.10, left panel), these fluctuations can influence the head end pressure (see Figure 3.2.10, right panel). We note that different propellant morphologies yield different head end pressure fluctuations, an observation impossible with traditional treatment of the propellant surface. We will continue this work in the coming fiscal year. This work is done in collaboration with F. Najjar.

**P7. Rocfire – Aluminized** The Rocfire version of the code described previously does not take into account aluminum. Since almost all solid propellants of interest contain some amount of aluminum, the code is being extended to include the necessary particle tracking and physics modules. The propellant surface and aluminum particles in the gas phase are tracked using level sets. Although the

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Fig. 3.2.10. Left: Instantaneous velocity contours (33% fluctuations) as function of normal distance above propellant surface; similar contours are obtained for temperature field (14% fluctuations about mean). Right: Head-end pressure as function of time for four different mass flux input distributions.

Fig. 3.2.11. Surface topography and temperature level-surfaces for sample propellant at instant of time (left) and 1.3 ms later (right).
P8. Agglomeration Modeling Here we discuss recent work on aluminum agglomeration, an important subject currently under investigation by both ATK and Aerojet. Typical solid rocket motor propellants, such as those used in the space shuttle boosters, are composed of ammonium perchlorate (AP) and aluminum (Al) particles embedded in fuel binder. A typical composition, by weight, is 71% AP, 18% Al, and 11% binder. The aluminum reacts exothermically with H$_2$O and CO$_2$ in the chamber, increasing the specific impulse by approximately 10%. It also provides efficient damping of chamber instabilities, a desirable effect. However, there are undesirable effects such as slag accumulation, nozzle erosion, and significant exhaust signatures. Because of these, aluminum behavior is one of the most important problems faced by the solid propellant industry. An essential feature is agglomeration of particles at the propellant surface. To this end we have developed an agglomeration model, based on Rocpack (see Figure 3.2.12, left panel), which yields both the agglomeration diameter and the agglomeration distribution (Figure 3.2.12, right panel), which are critical for meaningful simulations of nozzle and plume flows. The agglomeration model has recently been applied to a number of IHPRPT propellants developed at Aerojet West, and the results are extremely encouraging (Figure 3.2.12, right panel). The funding for Aerojet comes from the propulsion group at Edwards Air Force Base AFRL/PRS. We plan to further improve the agglomeration model in the coming fiscal year, and apply it all the data we can obtain from Aerojet and ATK Thiokol.

Project Plans A number of combustion projects critical to the overall success of Rocstar as a predictive tool for solid rocket motor simulations will continue in the coming fiscal year. The integration of Rational_Rochburn into Rocstar has recently been completed, and attempts will be made to develop a similar module for three-dimensional packs and for aluminized propellants. Rocpack is essentially complete, although we will build a GUI for the interface package Rocprep. Modifications to Rocpack to include the packing of three-dimensional elliptic cylinders might be considered if enough interest exists. The development of Rocfit is complete, and the coming fiscal year will see this important tool being applied to AP/HTPB propellants as well as more modern propellants of interest. Acoustics is an important problem, and if time allows we hope to revisit this problem for a more in-depth analysis, and to make it a module of Rocstar. The work on proper injection boundary conditions for meaningful LES simulations will continue to be an important problem. A module for stochastic injection boundary conditions was incorporated into Rocstar last fiscal year, and we expect further improvements in the coming fiscal year. Work on aluminized Rocfire will continue, the goal there being a fully functional three-dimensional version. We believe that one of the most important contributions that can be made here is to the agglomeration problem, one of enormous interest to the US
industry and of at least equal value to any Rocstar application. We are also examining the role of Alex (nanometer scale aluminum) in the combustion process, as there is considerable interest in this in the industry. The aluminum work and related issues (such as melt layers) could easily extend to the end of the current contract period, but we expect that interim results within the next year framework will be of fundamental value to the integrated code.