PERFORMANCE MODELING REQUIREMENTS FOR SOLID PROPELLANT ROCKET MOTORS*

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ABSTRACT

The purpose of this paper is to outline the engineering state of the art in combustion modeling of solid propellant rocket motors and to propose future improvements in the modeling tools used by the SRM community.

Currently there are three broad categories of models in use today. They are simple models where the entire combustion process is treated as a single entity, engineering models in which a portion of the combustion process is idealized and other parts are treated in detail, and finally full up and/or research models where all important combustion processes are modeled. Examples of these types of models are presented and recommendations for future model development are made.

INTRODUCTION

Over the pass decade there has been a growing realization within the solid propellant rocket motor community that the fine details of the combustion process inside the rocket engine or motor can have a first order effect on motor and nozzle performance as well as the observables in exhaust plumes. This realization has come about for many reasons, however, three major factors are:

- Failures of nozzles and inlets
- Lack of performance gains as predicted by standard models
- Improved measurements and diagnostics of combustion observables
- Improvements in the plume flowfield and radiation models
- Increased power and lower costs of computing resources

The purpose of this paper is to outline the engineering state of the art in combustion modeling and propose future improvements in the modeling tools used by the plume community.

Currently there are four broad categories of models in use today. They are simple models where the entire combustion process is treated as a single entity, engineering models in which a portion of the combustion process is idealized and other parts are treated in detail, and finally full up and/or research models where all important combustion processes are modeled. Some examples of these models are:

Simple models:
  Constant gamma equations (calorically perfect gas)
  Equilibrium chemistry solvers such as ODE[1], TEP[2], PEP[3], and CCET[4]
  Empirical models for burn rates, ignition delays, nozzle throat erosion, thrust losses, etc.

Engineering models:
  SPP[5] internal ballistics/performance prediction and SSP combustion instability codes
  SPP[5], VIPER[6], and NFM[7] nozzle flow codes

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[*] Approved for public release; distribution is unlimited.

Full up models:
- CELMINT[8] combustion chamber and nozzle flow solver
- GIFS[9] and CRAFT[10] nozzle and plume flow solvers

Research models:
- Solid propellant combustion models of Dr. Yang and his students at PSU
- Surface combustion models of Dr. Beckstead and his students as BYU
- CSAR SRM modeling of the staff at UIUC

Of the research models, only the CSAR SRM model attempts to treat the entire solid rocket motor.

One of the more telling features of these models is the data input requirement. The simplest models require only modest inputs that are generally available for domestic systems and estimable for foreign systems. Depending on the fidelity of the results desired, engineering model inputs could range from modest to requiring months of work in acquiring and understanding the necessary drawings and data. Full up models require all of the inputs of the more complex engineering models plus extra data, some of which can only be estimated. These data requirements are also true of the research models. However, the research models quite often require data that are just not available for most operational domestic systems. It is not unusual that sub-scale tests must be run to obtain the required data for both the full up and research models.

Another telling feature of these models is the expertise required to run the computer programs. Generally, junior level personnel can run the simple model with reasonable results. The engineering models require some training and experience in propulsion systems to analyze the more complex systems. Modeling of the detailed combustion process in either solid or liquid propellant systems requires great expertise. The full up models are best run by experts in propulsion analysis who are also very knowledgeable in CFD.

One of the most important considerations in modeling rocket propulsion systems is balancing the complexity of the model with the fidelity of the input data available. While not quite to the level of "*garbage in-garbage out*"[*], running high fidelity models with gross estimates for some of the key inputs makes little sense and can imply a level of accuracy which can be quite misleading. In the following sections, key input parameters are indicated. It is the determination of the input data available that should be one of our major guides to modeling decisions. Sometimes we can skirt around this issue by doing parametric studies over the plausible range of the unknown input parameters. However, parametric studies are difficult to do when the model takes a week to run on a high performance multi-processor computer systems.

In the end, it is the end user's intended use and requirements for data that is the final driver for model development. Real world constraints of budget, time, and availability of modeling resources must determine the selection of analytic, computational, statistical, or empirical models.

SOLID ROCKET MOTORS (SRM'S)

Solid propellant rocket motors cover such a giant expanse of shapes and sizes, propellants and system uses, that no simple description could do justice to the combustion modeling of them. Propellants and research models cover a broad range of oxidizers, binders, additives and the incorporation of energetic metal powders (chiefly aluminum). The rocket motors usually have a fairly rigid case with a liner and insulation to protect thermally sensitive parts, and may also have inert hydrocarbon components for ballistics (inhibitor) or structural (boot, retention, etc.) purposes. A small pyrotechnic ignition device is used to ignite the propellant grain, large motors use pyrogen type igniters, which are rapid acting small

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[*] Sometimes referred to as "garbage in-gospel out".

motors, initiated by pyrotechnics. The nozzles for most systems erode with time during the motor firing, and some systems employ unconventional nozzles (e.g., multiple nozzles, canted nozzles). The propellant grain can vary from simple 2-D geometries to quite complex 3-D configurations with varied insulation exposures. Tactical motors and even some strategic motors can employ dual-propellant designs. While the trend in strategic and launch systems is toward simpler grain designs, many tactical systems have quite complex shapes. Thrust termination schemes include blowout ports, complicated energy management systems, or just simple burnout.

DESCRIPTION OF THE COMBUSTION PROCESS

The combustion processes for solid propellants, both steady and non-steady are beginning to be well understood. This includes descriptions of the combustion of monopropellant oxidizers (AP, RDX/HMX, AN, etc.), monopropellant binders (nitrate ester, oxetane, azide types and plasticizer /polymer combinations), inert rubber-base binders (polybutadienes, polyethers, polyesters, etc.) and various combinations thereof in composite propellants.

Our knowledge of the burning of the aluminum and the formation of the metal oxide particles has improved dramatically over the past decade. Current theories suggest that the raw Al particles melt on the surface of the propellant and form puddles. Steamers of unburned Al are carried away from the surface with the combustion gases forming Al agglomerates. Aluminum oxide is formed when the molten Al burns. The oxidation process occurs on the surface of the particles and within the interior of agglomerates as well as in the aluminum vapor phase adjacent to the particles. This process generates a bimodal distribution of oxide particles, large ones from the surface/interior combustion of agglomerates (tens to hundreds of microns) and very small ones (smoke, on the order of 1 micron) from the vapor phase combustion. Some of the Al agglomerates burn out completely, some do not leaving a fraction of unburned aluminum. Most of the residual agglomerates join the fine smoke to flow out through the nozzle but many are large enough to depart from the exhaust gas flow and be retained to form slag that is trapped around submerged nozzles.

There are significant differences in the aluminum combustion behavior between the different types of propellants. Less desirable behavior tends to occur in low burn rate propellants and propellants which do not contain AP. But since agglomerates contain a large number of the starting Al particles per agglomerate, variations in properties of the starting aluminum which affect agglomeration (e.g., thickness of natural oxide coating, impurities) can affect the performance of the motor and amount of slag. It is the influence of small variations in propellant properties, which have a large effect on the combustion process that are not well understood.

GEOMETRICAL AND RELATED CONSIDERATIONS

Besides the combustion process, there are other things happening in an SRM which should be considered in detailed models. These events include changes in the solid propellant grain shape due to casting cool down and from pressurization of the case during motor start up. Grain deformation at start up includes both the case and the propellant itself. That grain deformation can radically effect the combustion dynamics of a motor what dramatically demonstrated by the failure of one of the first Titan SRMU motors.

The burning back of the propellant grain has a first order effect on the thrust time history of the motor. The major players in being able to model the burn back are grain shape, burn rate, and nozzle throat erosion. As mentioned before, cool down and pressure deformation can have a significant effect on grain shape. The propellant burn rate is a function of motor size, the way in which the propellant was cast (rheology or hump effect), and the motor flowfield (erosive burning). A reasonable model of how the nozzle throat area varies with time is necessary to match the measured thrust or pressure trace.

The internal geometry of the motor will have an obvious effect on the flow in the nozzle. Not only are there contributions from the grain geometry, but the length of the motor and the shape of the nozzle inlet will all have an effect on the flow field. Star shaped grains will cause flow patterns that can be traced back to star tips and valleys. The length of the grain will affect channeling of the particles entering the nozzle. The nozzle entrance, especially for submerged nozzles, has an impact on both the gas/particle flowfield and the particle size distribution. Other geometrical effects with time include insulation exposure and nozzle material ablation. Nozzle throat erosion has a major impact on the pressure and thrust time history of a motor.

The exposure and ablation of the motor liner and insulation material can affect the plume signature and base heating. Both of these materials are usually rubber based and are very good insulators. The good insulation characteristics cause the surface to heat up quickly to the ablation temperature and the carbon in the rubber results in carbonaceous ablation products that are introduced into the flowfield. These ablation products are good continuum emitters.

PARTICLE DYNAMICS

Of great interest for both performance prediction and plume flowfield/radiation calculations is the state of the particulate matter leaving the exhaust nozzle. In the description of the combustion process, it was noted that the particle size distribution was bimodal consisting of very large and very small particle sizes. The large particles, due to their higher mass, tend to travel slower that the fine smoke particles. This velocity difference causes the small particles to run into the larger ones and form even larger agglomerates. Once the large particles enter the nozzle entrance section, they are accelerated along with the flow. The acceleration forces coupled with the shear or drag force causes these large particles to breakup into smaller particles. Hence the distribution of particle sizes changes from bimodal to log normal. At some point in the expansion process, the temperature of the particles drops below the freezing point of the liquid alumina and a crystallization process begins from the surface of the drop inward.

The drag on the particles ranges from Stokes' flow in the chamber to free molecular in the exhaust nozzle. Also, there is a large variation in alumina properties during the expansion, which should not be ignored.

NOZZLE FLOW AND MOTOR TRANSIENTS

In addition to the two phase flow effects discussed above, particular mechanisms of interest to solid propellant nozzle flows which call for more detailed analyses are non-uniform entrance conditions due to grain design, insulation fuel flow in the nozzle boundary layer, and alumina agglomerate break-up. The insulation and related hydrocarbon internal components of the motor are important to the survival of the thermal protection system and are becoming recognized as important in plume phenomena. Also required for SRM's is the ability to treat steps in the nozzle wall and 3-D flow due to multiple nozzles being fed from a single combustion chamber.

There are several notable transients for SRM's. These include ignition and shut down transients, thrust vector control, and scheduled thrust variations. The ignition transient is important since it controls the flame spreading of the grain and the overpressurization of the motor case. The igniter quite often has a different propellant than the motor. Other than that, the ignition transient has only a minor effect on either nozzle performance.

Motor thrust variations and shut down have an obvious impact on the plume signature. In a large number of cases, varying the thrust has a very minimal impact on Isp and hence chamber pressure/flow rate scaling can be used to calculate the thrust and nozzle exhaust products. In other cases, the combustion efficiency can change and a new point analyses are required. For larger engines, throttling can almost always be modeled as a quasi-steady event. The major problem with dealing with motor shut down is that chuffing can occur as the propellant extinguishes and then re-ignites.

There are a number of thrust vector control methods used in solid propellant motors. These include various flex seals, Liquid Injectant Thrust Vector Control (LITVC), and thrust defection such as jet vanes, jet tabs or jetavators. Flex seal methods have the least effect on nozzle performance and it is quite often assumed that there is no effect on the gases entering the nozzle. The slewing rate for flex sealed nozzles is usually slow enough that a vacuum plume would not be affected. LITVC injects a fluid into the supersonic portion of the nozzle where a shock wave and induced boundary layer separation occur. The shock increases the pressure on the nozzle wall asymmetrically, which in turn produces the vectoring moment. The injectant is usually very energetic and will produce a pronounced perturbation to the plume.

SUMMARY AND RECOMENDATIONS

So far we have discussed the phenomena and technical elements which should be considered in computerized models for solid propellant rockets. The complexity of the models has been broken down into three categories, simple, engineering, and full up. Given below is a short summary of what we think should be contained in a complete model within these categories followed by our recommendations as to what technical elements should be developed first and how. Also, it should be pointed out that at this time no nozzle codes exist that meet the criteria we have laid out for any of the three categories.

SIMPLE MODEL

The simple model requirements that have been laid out are worth implementing in a computer program. Such a code would allow for the quick and simple estimation of motor/engine performance and plume starting conditions. In addition, by incorporating the experiences of senior engineers within the code, junior personnel will be able to achieve better results with a reduced learning curve. A simple model is especially appropriate for poorly characterized foreign systems. The simple model can be developed completely independently of the more advanced computer models and should contain the recommendations we have made for solid propellant systems. To summarize, the simple model should contain:

Performance Using Equilibrium Thermochemistry
    Shifting equilibrium
    Frozen flow starting from chemical equilibrium
    Shifting equilibrium to a sudden freeze point
    Finite area combustion
    Ability to specify a fraction of soot or other combustion product
    Ability to specify an unburned constituent
    Air-augmented burning to simulate ducted rockets and/or afterburning

Loss Models
    Combustion efficiency (C*) correlation
    Divergence loss (cosine half-angle law)
    Performance delivered to variable atmosphere conditions
    Other loss correlations, e.g., two-phase flow, boundary layer, kinetics, etc.

Motor Model
    Pressure vs. time or web, simple lumped volume internal ballistics module which uses simple 2-D grain shapes or input tables of geometry versus web
    Burn rates
    Nozzle throat erosion correlation

In addition, the simple code should contain users friendly features such as libraries of propellants, grain shapes, material properties, and sample cases of known non-classified systems.

ENGINEERING MODEL

The engineering model represents an almost complete analysis tool for evaluating the performance and plume starting conditions for rocket motors. An attempt has been made where possible to balance the fidelity of the input data requirements with the model accuracy. Some phenomena have been left out as being too complex or requiring too much data that are not usually available for an engineering analysis tool. Computer run times were also a criteria in determining if a phenomena should be included or not. However, we have strived not to leave out any first order effects in predicting the performance of these systems for any reason. We have also tried to include at some level all of the known important factors required for determining the starting conditions for the exhaust plume flowfield and its resultant emissions. To summarize, the engineering model should contain:

SRM Motor Phenomena

Motor/Combustion Chamber

- Grain design
  - Grain burnback and insulation exposure
    - Generalized 3-D multi-perforated propellant grains
    - Single propellant with anomalies
    - Dual propellant
    - Coupled and uncoupled with internal ballistics
  - Grain deformation
    - Cool down
    - Pressure loads
- Internal ballistics
  - Gas/particulate addition due to a simple burn rate law
  - 1-D quasi steady flow with variable gas properties for 2 propellants
  - Erosive burning
  - Igniter mass flow/ignition transient
  - Pressure drop for radial slots
  - Insulation mass flow and soot fraction computations
  - Particulate/discrete phase flow with finite dynamic and temperature lags
  - Particle agglomeration and breakup
- Nozzle throat erosion
  - Both simple correlation and thermochemical erosion/ablation calculation
- Propellant combustion
  - Base burn rate
  - Modifications to base burn rate for dp/dt transient and erosive burning effects
  - Agglomerate size prediction, size distribution of particles emanating from the propellant surface
  - Computation of amount of unburned aluminum
  - Fraction of soot from propellant binder (in addition to insulation contribution)-

- Combustion Instability Option
  - Computation of acoustic modes coupled to grain design module
  - Propellant response functions
    - Coupled to internal ballistics module
  - Particle damping losses
    - Coupled to aluminum behavior computations, or uncoupled
    - Stability additive contributions
  - Nozzle damping losses
    - Coupled to internal flow and nozzle erosion computations, or uncoupled
  - Other acoustic losses

SRM Nozzle Flowfield Phenomena

- Nozzle inlet, throat, and exhaust nozzle
    - Nozzle inlet and throat
        - Gas-particle coupled solution including all of the elements listed under “Two phase flow”
        - Uncoupled perturbation solution of the type used in SPP/VIPER
- Two phase flow
    - Real gas properties
    - Particulate/discrete phase flow with finite dynamic and temperature lags
    - Particle accretion and breakup
    - Particle non isothermal solidification model
    - Particle drag model (at a minimum: Crowe, Henderson, or Hermsen model)
    - Particle size model
- Finite rate chemistry
    - Global reactions
    - Binary exchange and third body reactions
    - Soot formation and oxidation
    - Excited state chemistry
- Viscous flow
    - Wall shear layer
    - Wall heat transfer
        - Ablative cooling
        - Adiabatic wall
        - Specified wall temperature
        - Radiation cooled wall
- Exhaust nozzle
    - Ability to handle the actual nozzle geometry in at least a 2-D or axisymmetric manner

FULL UP MODEL

The full up model represents as complete an analysis tool for evaluating the performance and plume starting conditions for rocket motors and engines as is feasible for use on a regular basis. An attempt has been made where possible to balance the fidelity of the input data requirements with the model accuracy. Some phenomena have been left out as being too complex, not well enough understood, or requiring too much data that are not usually available. Computer run times were only a minor consideration for selecting phenomena. We have tried to include at some level all of the known important factors required for determining the starting conditions for the exhaust plume flowfield and its resultant emissions. To summarize, the full up model should contain:

SRM Motor Phenomena

Motor/Combustion Chamber

- Grain design
    - Grain burnback and insulation exposure
        - Generalized 3-D multi-perforated propellant grains
        - Single propellant with anomalies
        - Dual propellant
        - Coupled and uncoupled with internal ballistics and including anisotropic burning rates
    - Grain deformation
        - Cool down
        - Pressure loads
- Internal ballistics

        - Gas/particulate addition due to a simple burn rate law
        - 1-D quasi-steady flow with variable gas properties for 2 propellants
        - Erosive burning
        - Igniter mass flow/ignition transient
        - Pressure drop for radial slots
        - Insulation mass flow and soot fraction computations
        - Particulate/discrete phase flow with finite dynamic and temperature lags
        - Particle agglomeration and breakup
        - 2 and 3-D quasi-steady flow field calculations
    - Nozzle throat erosion
        - Both simple correlation and imbedded thermochemical erosion/ablation calculation
    - Propellant combustion
        - Base burn rate
        - Modifications to base burn rate for dp/dt transient and erosive burning effects
        - Agglomerate size prediction, size distribution of particles emanating from the propellant surface
        - Computation of amount of unburned aluminum
        - Fraction of soot from propellant binder (in addition to insulation contribution)
        - Anisotropic burning models for casting rheology effects and designed burn rate variations (wires or foam insets)
    - Combustion Instability Option
        - Computation of acoustic modes coupled to grain design module
        - Propellant response functions
            - Coupled to internal ballistics module
        - Particle damping losses
            - Coupled to aluminum behavior computations, or uncoupled
            - Stability additive contributions
        - Nozzle damping losses
            - Coupled to internal flow and nozzle erosion computations, or uncoupled
        - Other acoustic losses

SRM Nozzle Flowfield Phenomena

- Nozzle inlet, throat, and exhaust nozzle
    - Nozzle inlet and throat
        - Gas-particle coupled solution including all of the elements listed under “Two phase flow”
        - Uncoupled perturbation solution of the type used in SPP/VIPER
    - Two phase flow
        - Real gas properties
        - Particulate/discrete phase flow with finite dynamic and temperature lags
        - Particle accretion and breakup
        - Particle non isothermal solidification model
        - Particle drag model (at a minimum: Crowe, Henderson, or Hermsen model)
        - Particle size model
    - Finite rate chemistry
        - Global reactions
        - Binary exchange and third body reactions
        - Soot formation and oxidation
        - Excited state chemistry
    - Viscous flow
        - Wall shear layer
        - Wall heat transfer
            - Ablative cooling
            - Adiabatic wall
            - Specified wall temperature
            - Radiation cooled wall

Exhaust nozzle

Ability to handle the actual nozzle geometry. Includes non-circular throats, steps in the wall geometry, and multiple nozzles.

Our recommendations are based on our knowledge and engineering judgement of rocket propulsion systems. It is also based on our experience in developing similar large engineering software systems. If we are not to make the mistakes that have plagued similar development programs, we must follow the guidelines given below.

- Realistic goals and schedules must be established with adequate funding. Unrealistic goals almost always lead to large cost overruns coupled with significant technical under-runs.

- Testing of the component software by organizations other than the developers is required along with peer review of both the models and implementation methods. Early delivery of the software to the user community leads to better and more robust software. While no one likes to be criticized about a work in progress, the developers of the software will just to have to put up with criticisms, justified or not. Programmatic review by a steering committee, while necessary, should not be confused with peer review.

- Maximum use of existing software is required in order to deliver complete or near complete software to the user community in a reasonable time frame. Modern FORTRAN compilers allow legacy code to be modularized and segregated (encapsulated) from newer code. This practice allows existing models to be used without contaminating the new code being developed. The interface requirements for the models are generally driven by the physics involved and not by the implementation. Legacy models can be replaced at a later time without a loss of generality.

- The requirements for good mesh generators, graphical analysis and displays, and generalized data management will best be met if commercial off the shelf (COTS) software is extensively used. The use of COTS software will increase the utility and robustness of the system while lowering the development cost.

- Computer codes require maintenance just as do jet planes and automobiles. A commitment to maintain the codes developed should be made at the outset of the development effort.

It is anticipated that the model requirements outlined here will lead to the development of new software at some future time. It is our recommendation that the development start with the simple model system and progress to the engineering model. Since it very likely that these models will be incorporated into a more complex system analysis software package, the interface between the nozzle combustion codes and the systems code can be worked out at an early stage in the development cycle. This approach allows not only for a top down design but also a top down implementation. It is also recommended that a version of the simple model be developed as a stand-alone package with a user friendly graphical user interface.

The development of the engineering model is a major piece of work even with the maximum use of existing software.

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