**Title:** A Model of the Effects of Pressure and Crossflow Velocity on Composite Propellant Burning Rate

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A MODEL OF THE EFFECTS OF PRESSURE AND CROSSFLOW VELOCITY ON COMPOSITE PROPELLANT BURNING RATE

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Abstract

Several variations of a model for prediction of burning rate versus pressure behavior of unimodal oxidizer composite propellants in the absence of crossflow were developed and evaluated against a set of data for a series of four formulations. Three variants, including one in which an average oxidizer-burning-surface intersectional area concept is employed and two in which allowance is made for geometry and stoichiometry changes as the propellant recedes past an oxidizer crystal, were found to give excellent agreement with data. The former variant was extended to treat multimodal oxidizer formulations, yielding predictions in excellent agreement with data for two additional formulations containing bimodal oxidizer. In the initial development of the erosive burning aspect of the model, columnar diffusion flame bending was assumed to be the sole mechanism leading to burning rate augmentation by crossflow: this assumption led to severe underprediction of erosive burning effects. Accordingly, the model was revised through addition of a flow profile analysis for prediction of cross-flow-induced turbulence augmentation of transport properties governing heat feedback from gas flames as well as flame-bending. This revised model was found to yield good agreement with erosive burning data for five of the six formulations tested, but gave higher predicted rates than observed values for the sixth propellant.

Introduction and Background

Erosive burning, the augmentation of solid propellant burning rate by the flow of products across a burning surface, is becoming increasingly important with use of lower port-to-throat area ratio motors and nozzleless motors, both of which result in high velocity crossflows. The response of various propellants to such crossflows must be known by the motor designer in order for him to perform adequate motor design. In addition, it is important that the propellant formulator understand the effect of various formulation parameters on the sensitivity of a propellant to crossflow so that he may tailor his propellants to the desired characteristics. For example, in a nozzleless rocket motor, the decrease in pressure from the head end to the aft end of the grain tends to result in slower burning at the aft end in the absence of erosive effects. Depending upon the sensitivity of the formulation to crossflow, the increasing Mach Number along the grain port may lead to undercompensation, exact cancellation, or overcompensation of the pressure effect. A detailed discussion of the effects of erosive burning on solid propellant rocket interior ballistics for low port-to-throat area ratio motors and nozzleless motors was presented by this author in Reference 1. During the past three years, this author has been conducting an analytical and experimental study of the erosive burning of composite propellants. This effort includes: (1) development of a simplified model for prediction of the erosive burning of a composite propellant, given the non-erosive burning rate versus pressure relationship for that formulation; (2) development of a more fundamental composite propellant combustion model for prediction of burning rate as a function of pressure and crossflow velocity, given only the propellant composition and ingredient particle size distributions; (3) experimental measurement of the erosive burning characteristics (at crossflow velocities up to Mach 1) of a series of propellants with systematically varied compositions and ingredient particle sizes; and (4) fine tuning of the models using this experimental data. The simplified (Generation 1) model has been described in detail in References 2 and 3, with the experimental procedure and test results to date appearing in References 3 and 4.

Details of the first variant of the more fundamental (Generation 2) model for the prediction of burning rate as a function of pressure and crossflow velocity appear in Reference 5. (That reference will be cited heavily throughout this paper, with later variants of the Generation 2 model being described in terms of modifications of the analysis presented therein.) This first variant of the Generation 2 model employs many of the concepts used in the Beckstead-Derr-Price (BDP) composite propellant combustion model(6) with, however, major modifications, including:

1. Variation in the ratio of local oxidizer-surface intersectional area to the binder surface area as the propellant surface regresses past an oxidizer particle is considered. (In the BDP model, a geometrical average ratio is used; this involves an assumption that a lot of very nonlinear processes can be linearly averaged. In tracking the regression of the flame front through an oxidizer crystal in this first model variant, one finds a strong variation in local flame temperature, stoichiometry, and diffusion flame dimensions between polar and equatorial intersections, as discussed in detail in Ref. 5.)

2. The kinetics of subsurface/surface exothermic reactions are considered, with use of rate expressions based upon the work of Waesche and Wenograd.(7) (In the BDP model, subsurface/surface heat release is included with the endothermic ingredient vaporization heats, with the resultant implicit assumption that the amount of heat release in these reactions per unit mass of propellant is independent of such parameters as burning rate.)

3. A correction of an inconsistency in definition of areas in the BDP model is made.
4. The calculation of the dimensionless stoichiometric group needed for calculation of the diffusion flame height via the Burke-Schumann analysis is modified. (The group used in the BDP model is inconsistent with that defined in the original work of Burke-Schumann.)

5. A two-flame (fuel-gas/oxidizer-gas columnar diffusion flame and ammonium perchlorate monopropellant flame), rather than a three-flame model, is used. (With correction of the calculation of the stoichiometry dimensionless group for the Burke-Schumann analysis, it no longer appears necessary to differentiate between the parts of the diffusion flame inside and outside of an ammonium perchlorate monopropellant flame.) (See Figure 1.)

6. The procedure for calculation of heat feedback from the diffusion flame and the AP monopropellant flame is modified. (In the BDP model, all flames are considered to occur in flame sheets at discrete distances from the surface; in the current model, the AP monopropellant heat release is treated as a flame-surfact type heat release but the diffusion flame heat release is considered to occur in a distributed fashion over a finite range of distances from the propellant surface.) (See Fig. 1.)

7. The distance (measured normal to the propellant surface) associated with oxidizer-binder gas interdiffusion in the presence of crossflow is assumed to be reduced by a factor, sin θ, where θ is the angle of the resultant of the crossflow and burning rate is zero. (Since the oxidizer and fuel in general regress at different rates, it is possible for an oxidizer particle to burn out before the binder reaches the bottom of its associated pit, leading to zero burning rate for the remaining increments, as discussed in Ref. 5.)

As mentioned earlier, details of the development of the first variant (baseline) of the Generation 2 model are presented in Reference 5. The basic units of the model construction consist of development of a procedure for description of the surface structure at succeeding incremental steps of regression of the binder past an oxidizer particle, application of an energy balance at the surface along with numerous ancillary equations at each increment for calculation of burning rate at that increment, and averaging of the incremental burning mass fluxes to obtain an overall average burning rate. In this baseline variant, an organized crystal array was assumed and used to calculate the relative planar oxidizer and fuel areas at each intersection depth. As discussed in some detail in Ref. 5, choice of the best procedure for calculating an average rate (the "end-game" procedure) is not clear; several averaging equations are presented. The procedure chosen for use with the first variant of the model was:

\[ \bar{F}_{\text{avg,propellant}} = \frac{1}{p_{\text{propellant}}} \sum_{\text{j}} \left( F_{\text{OX,AP,}j} + F_{\text{fuel,AFU,j}} \right) \]

with the summation being carried out over all increments, including ones for which the mass efflux rate is zero. (Since the oxidizer and fuel in general regress at different rates, it is possible for an oxidizer particle to burn out before the binder reaches the bottom of its associated pit, leading to zero burning rate for the remaining increments, as discussed in Ref. 5.)

As explained in detail in References 2-5, a mechanism by which crossflow is postulated by this author to affect the burning rate of composite propellants involves the shortening of the distance (measured normal to the surface) associated with the mixing of columns of fuel and oxidizer gas leaving the propellant surface. In the combustion of ammonium perchlorate-loaded composite solid propellants, it is generally accepted that parallel columns of oxidizer and binder sublimation/decomposition products leave the surface from above the oxidizer crystals and binder, respectively. In the most general case some heat is fed back to the surface from monopropellant reaction of oxidizer sublimation products while additional heat is supplied by the mixing and reaction of the oxidizer and fuel product streams. (Fig. 1.) Accordingly, an important factor in determining the rate of heat feedback which increases with decreased distance of the gas-phase heat release zone(s) from the surface is often the rate of mixing of the oxidizer and binder gas product columns. In the absence of a crossflow, these columns move perpendicular to the propellant surface, while, with crossflow, they are tilted over and travel at an angle to the surface, this angle being determined by the ratio of crossflow velocity to transpiration velocity at any given position above the surface. As a result of this bending, the mixing distance, measured perpendicular to the surface, decreases. A particularly detailed description and explanation of this postulated mechanism is presented in Ref. 3 and 4. In the development of the Generation 1 model and in the early stages of development of the Generation 2 model, this mechanism was assumed to be the only factor causing composite propellant burning rate to increase in the presence of a crossflow.

During the past year, several additional variants of this second-generation model have been developed in a search for an optimum model, both in terms of fundamental physics and in terms of explaining experimental observations regarding the effects of such parameters as pressure, oxidizer particle size, and propellant composition on burning rate. In addition, one of the variants was extended to handle multimodal oxidizer formulations. The original erosive burning section of the Generation 2 model was found to be inadequate, as discussed later, and this section was subsequently modified (in this same variant) to allow for augmentation of gas-phase transport properties by crossflow-generated turbulence as a second erosive burning mechanism. The variants examined are summarized in Table I, and details of the modifications of the original baseline variant (described in detail in Ref. 5) to yield these latter variants are presented in the next section, along with a description of the extension of the selected variant (IV) to handle multimodal oxidizer cases and to treat crossflow-induced turbulent transport property augmentation. Comparison of predictions and data are then presented in the following section.

Model Development

Unimodal Oxidizer, No Crossflow

As indicated above, the first (baseline) variant of the Generation 2 model is described in detail in Reference 5. Nomenclature used in the following model descriptions is consistent with that used in that paper to facilitate comparison. The sole difference between Variant I and Variant II lies in replacement of the procedure of following the receding binder in incremental steps past the oxidizer crystal with use of an "average burning surface-
oxidizer intersection" concept similar to that used by Beckstead, Derr, and Price. (6) (This is, of course, a major simplification to the model since the surface energy balance and ancillary equations described in Ref. 5 need now be solved only once rather than a number of times equal to the number of incremental steps considered in the baseline variant, generally 20 or more. Similarly, the geometric relationships describing the surface only have to be solved once rather than being recalculated sequentially at each increment.) As in the baseline variant, the fuel is assumed to regress in a planar manner and the oxidizer-fuel surface is forced to be continuous at their intersection.

These restrictions, coupled with the fact that the linear regression rates of fuel and oxidizer perpendicular to their directions of regression are allowed to differ, force the oxidizer to in general assume a curved shape as it regresses, thus creating additional burning area. As in the BDP model, upper hemisphere and lower hemisphere average intersections are considered and values of the curved oxidizer areas (APOX) are calculated at each intersection and averaged together. The "average" intersection in each hemisphere is defined such that the planar oxidizer-burn surface intersectional area (APOX) is the average of the areas of all possible intersections in that hemisphere. With application of geometrical analysis and continuity relationships, it is easily shown that:

\[ A_{\text{POX}} = \pi d_o^2 / 2 \]  
(2)

\[ A_{\text{FU}} = (\pi d_o^2 / 6) (1 - \ln \theta) / \theta \]  
(3)

In addition, the distances from the initial top of the oxidizer particle to the fuel surface at the upper and lower intersections can be shown to be

\[ D_{\text{TOP Upper}} = (d_o / 2) (1 - \sqrt{3}) \]  
(4)

\[ D_{\text{TOP Lower}} = (d_o / 2) (1 + \sqrt{3}) \]  
(5)

Assuming no ignition delay for the oxidizer particle, the corresponding distances from the initial oxidizer peak to the center of the oxidizer crystal at the times when Eqs. 4 and 5 are satisfied are:

\[ D_{\text{OX Upper}} = \left( \frac{r_{\text{OX}}}{r_{\text{Fuel}}} \right) D_{\text{TOP Upper}} \]  
(6)

\[ D_{\text{OX Lower}} = \left( \frac{r_{\text{OX}}}{r_{\text{Fuel}}} \right) D_{\text{TOP Lower}} \]  
(7)

(with restraints that \[ D_{\text{OX}} < D_o \].) Again through geometrical arguments, it may be shown that

\[ ASOX_{\text{Upper}} = \pi D_o^2 \left[ \frac{1}{2} - \frac{1}{\sqrt{3}} \right] \left[ 1 - \left( \frac{2 D_{\text{OX Upper}}}{D_o} \right)^2 \right] \]  
(8)

\[ ASOX_{\text{Lower}} = \pi D_o^2 \left[ \frac{1}{2} + \frac{1}{\sqrt{3}} \right] \left[ 1 - \left( \frac{2 D_{\text{OX Lower}}}{D_o} \right)^2 \right] \]  
(9)

In Variant II of the second generation model, Eqs. 2 - 9 are used to calculate APU and ASOX values to replace those used in Variant I. In addition, the time-dependent flame temperature and gas heat capacities of Eqs. 32 and 33 in Ref. 5 are replaced by values corresponding to the overall propellant stoichiometry. Finally, the burning rate is calculated as:

\[ r_{\text{avg}} = \frac{r_{\text{OX}} (ASOX)}{APOX} \]  
(10)

(replacing Eqn. 35 of Ref. 5).

Variant III differs from Variant I in several ways, all of which are believed to entail more realistic descriptions of various processes occurring during the burning of a composite propellant. First, the dependence of the O/F flame kinetic distance, \[ L_{\text{OX}} \], on the flame temperature was changed from that given by Eqn. 25 in Ref. 5 to:

\[ L_{\text{RX}} = \frac{K_{\text{OP RAS surf}} (1 + \eta^2) \exp \left[ \frac{E_{\text{ACT OP/RT}}}{\rho (n-1)^{1/2}} \right]}{p (n-1)^{1/2}} \]  
(11)

and the corresponding oxidizer flame kinetic distance was altered from Eqn. 26 (Ref. 5) to:

\[ L_{\text{AP}} = \frac{K_{\text{AP surf}} \exp \left[ \frac{E_{\text{ACT AP/RT}}}{\rho (n-1)^{1/2}} \right]}{p (n-1)^{1/2}} \]  
(12)

to allow dependence on local temperature (which is calculated in a trial-and-error loop on the basis of position of the AP flame relative to the beginning and end of the diffusion flame). In addition, the analysis of subsurface heat release was modified to allow reaction only in the liquid melt layer near the surface and to allow for reactant depletion (first order kinetics) with resultant replacement of Eqn. 20 in Ref. 5 by:

\[ a = 1 - \exp \left( -\int ZINT \right) \]  
(13)

\[ B_{\text{sub melt}} \exp \left[ \frac{E_{\text{ACT sub}}}{\rho (n-1)^{1/2}} \right] \]  
(14)

\[ U_L = - \ln \frac{T_{\text{melt}} - T_o}{T_s - T_o} \]  
(15)

for \( T_s > T_{\text{melt}} \)

Finally, the assumption in Variant I that the O/F flame heat release is uniform between \( y = L_{\text{OX}} \) and \( y = L_{\text{OX}} + \pi \theta d_0 \sin \theta \) was replaced with a distributed heat release more heavily weighted toward the base of the diffusion flame, this weighting determined by detailed mixing profiles calculated via the Burke-Schumann(8) analysis. This resulted in replacement of Eqs. 22 and 23 of Ref. 5 with considerably more complex expressions for heat feedback fluxes from the gas-phase flames.

As indicated in Table I, Variant IV is the same as Variant III except for use of an "average intersection" concept; thus, modification of Variant III to Variant IV follows exactly the same procedure as the modification of Variant I to Variant II, described earlier.

Variants V and VI represent modifications of Variant III to allow different surface temperatures for the binder and oxidizer. To permit this, separate energy balances are written for the oxidizer and binder (replacing Eqn. 34 of Ref. 5), with the oxidizer receiving feedback from the oxidizer monopropellant flame and the diffusion flame, while the binder receives feedback only from the diffusion flame. The diffusion flame feedback is apportioned between binder and oxidizer in the ratio of the planar fuel and oxidizer areas. Subsurface heat release is apportioned so that the oxidizer receives
the fraction, \(1/(1 + \text{SRB0})\), while the binder receives the fraction \(\text{SRB0}/(1 + \text{SRB0})\), where \(\text{SRB0}\) is the stoichiometric ratio (mass) of binder to oxidizer. The only difference between Variants V and VI is in the treatment of the effect of non-planar surface structure on gas flame standoff distances relative to the oxidizer surface. In Version V, allowance is made for the non-planar structure. For oxidizer protruding, the distance from the oxidizer surface to the outer edge of the O/F flame is reduced by the average protrusion height. For oxidizer recessed, the distance from the oxidizer surface to both the inner and outer edges of the O/F flame is increased by the average recession depth. In Version VI, no such adjustment is made, it being assumed that the flame is wrinkled in such a manner as to track the surface contour.

Variants IIIA, IIIB, and IIIC all represent modifications of Variant III aimed at increasing the predicted dependence of burning rate on overall propellant flame temperature. (As will be discussed later, the strong variation of flame temperature with increment location in Variant III causes the effect of overall average flame temperature to be fairly well washed out in application of that variant.) Variant IIIA is quite similar to Variant III except that O/F flame temperature (\(T_f\)) and gas heat capacity (\(C_p\)) values corresponding to the local oxidizer/fuel ratio at each increment (as expressed by Eqsns. 32 and 33 in Ref. 5), we use flame temperature and heat capacity values equal to the overall propellant flame temperature and gas heat capacity, independent of increment number, at each increment. That is, Eqsns. 32 and 33 of Ref. 5 are replaced by:

\[
T_f = T_f^0 (1 - \text{WFO}) \tag{16}
\]
\[
C_p = C_p^0 (1 - \text{WFO}) \tag{17}
\]

where the functionalities are generated by application of a thermochemical equilibrium calculation.

Consistent with this modification, we also slightly modify the "end-game" procedure of calculating the overall propellant linear burning rate from the mass flux values calculated at each incremental intersection. Equation 1 of this paper is still employed, but the intersections are now limited to incremental intersections for which the mass fluxes are non-zero. (That is, increments corresponding to "outside" burner are not considered, with the assumption being made that the residual binder "breaks off" in some manner.) This has no effect on the numerator of Eqn. 1, but lowers the value of the denominator in cases where the oxidizer recedes more rapidly than the binder. (This modification of the "end-game" procedure is consistent with the use of flame temperature equal to overall propellant flame temperature at each incremental intersection in that such use implies an oxidizer/fuel ratio in the final flame equal to the overall propellant oxidizer/fuel ratio, thus implying that the "left over" binder is indeed somehow fed into the flame. It must be emphasized that this is not a closed question, however. As discussed in Ref. 5, definition of an optimal "end-game" procedure for calculation of an average linear propellant regression rate from values calculated at various points in the passing of the burning front through an oxidizer particle is somewhat nebulous, at best.)

Variant IIIB is also a derivative of Variant III, with arbitrary assignment of fuel to oxidizer at various incremental intersections according to:

\[
\text{AFU} = C_p \left( \text{DOX}/\text{XNA} \right) \tag{18}
\]

where XNA is an arbitrary input constant and \(C_p\) is determined for a given value of XNA by consideration of overall continuity for the propellant. A value of XNA = 0 corresponds to the ratio of fuel to oxidizer participating in the fuel-rich regions of the oxidizer at each intersectional area being independent of increment number, while XNA\textless{}0 results in polar intersections burning more fuel-rich than equatorial intersections. As will be discussed later, this variant showed very little promise for values of XNA between 0 and -1, and was quickly discarded.

In Variant IIIC, still another offshoot of Variant III, the oxidizer/fuel ratio of gas streams associated with a given oxidizer particle at each intersection depth was forced to be the same, equal to the overall propellant oxidizer/fuel ratio. This was accomplished by adjusting the fuel area associated with the oxidizer at each intersection depth in accordance with:

\[
\text{AFU} = \left( \frac{\text{OX}_j}{\text{OX}_j^0} \right) \text{DOX} \tag{19}
\]

This modification corresponds to doing away with the concept of an organized matrix of oxidizer crystals in the binder matrix, employed in Variants I, III, V, VI, and IIA (and described in detail in Ref. 5), and replacing it with the assumption that random distribution of oxidizer crystals results in the average O/F characteristics of a polar intersection (averaged over all polar intersections) and the average O/F characteristics of an equatorial intersection being the same. Among other things, this approach has the pleasing effect of eliminating the problem of "leftover" binder which crops up with the other variants. In addition, the average linear propellant burn rates calculated using the different averaging procedures described in detail in Ref. 5 are more nearly equal in this variant than in the other variants considering incremental passage of the burning surface through an oxidizer particle. Further, as will be discussed later, this variant is much more successful than Variant III in predicting dependency of burn rate on overall propellant oxidizer/fuel ratio (and thus flame temperature). A different means of calculating average burn rate from the individual incremental rates (Eqn. 27 in Ref. 5) was found to give slightly better results than the procedures used in the other model variants. In this procedure, the burning rate is calculated by dividing the oxidizer particle diameter by the sum of the times required for consumption of each thickness until the bottom of the oxidizer particle is reached:

\[
\tau_{avg} = \frac{D_i^j \tau_{j}^j}{\sum_{j} \left( \text{DELOX}^j \right) / \text{OX}_{j}} \tag{20}
\]

To this author, this is another plus point for this variant since Eqn. 20 seems to be more physically realistic than Eqn. 1 for calculation of the average linear regression, though it did not produce satisfactory results in the other variants studied.

**Multimodal Oxidizer, No Crossflow**

As will be discussed later, Variants IIIA, IIIC, and IV were all found to give satisfactory results when tested against no-crossflow burning rate data for a series of four unimodal oxidizer composite propellants. Although Variant IIIC is the most appealing to this author on a physical basis, the
considerably lower computational complexity associated with Variant IV led to its selection for extension for multimodal oxidizer cases. This extension was carried out in a very straightforward manner using Glick's "petit ensemble" approach (9), in which a propellant containing oxidizer particles of different sizes is broken into a series of subpropellants or "pseudopropellants", each of which contains oxidizer of only one size. These subpropellants are assumed to burn non-interactively, with the unimodal oxidizer model being used to calculate a mass flux for each, and straightforward averaging according to fractional surface areas associated with each subpropellant then being used to obtain an overall propellant average linear regression rate. The only manner in which oxidizer of one size is allowed to affect the burning of a subpropellant containing oxidizer of another size is through possible influence on the assignment of fuel to that subpropellant. That is, rather than permitting calculation of eddy viscosity (and, by analogy, total effective thermal conductivity and diffusivity) as a function of distance from the propellant surface for a given crossflow velocity, transpiration velocity (determined by the propellant burning rate), and temperature field (dependent on the location of gas-phase heat release zones) was developed and coupled with the Variant IV combustion model for erosive burning calculations. An improved calculation of diffusion flame-bending angle was also incorporated in this analysis.

For this analysis, preliminary estimates of the burning rate (and thus transpiration velocity) and the distance from the surface to the end of the diffusion flame (\(L_{PX} + FH_90 \sin \theta\)) were first made using laminar transport properties as in the original erosive burning package. The nonblowing skin friction coefficient was then calculated as the maximum of a value calculated using a smooth-wall equation and one calculated using a rough-wall equation:

\[
C_{fo} = 0.95 \left[ 4 \log_{10} \left( \frac{Re}{k} \right) + 3.48 \right]^{-2}
\]

A blowing parameter, \(b\):

\[
b = \frac{2 \Delta T_{INJ}}{C_f/C_{fo}}
\]

was then calculated from the previously estimated burning rate and the freestream velocity. This parameter was next used to estimate the actual skin friction coefficient with blowing (transpiration). Unfortunately, there is essentially no data available for values of \(b\) greater than 6 - 8, and our range of interest tends to go to much higher blowing ratios. Accordingly, several different expressions were fit to existing data (10-14) and built into the program for optional means of calculating skin friction with blowing:

\[
C_{f/x_{fo}} = \exp \left[ -0.357 b + 0.0068 b^2 \right], b \leq 26.25
\]

\[
C_{f/x_{fo}} = \exp \left[ -0.5513 b + 0.01316 b^2 \right], b > 26.25
\]

\[
C_{f/x_{fo}} = \exp \left[ -0.576 b \right], b \leq 20
\]

\[
C_{f/x_{fo}} = b / (\exp(b) - 1.0), b > 20
\]

Next, the wall shear stress was calculated as:

\[
\tau_{avg} = \left( \frac{1}{\rho_{ax}} \right) \frac{\tau_s}{\rho_{ax}} \left( \frac{d_{ax}}{\rho_{ax}} \right)^2
\]
Application of a momentum integral analysis for a two-dimensional channel (the configuration in which testing was conducted) yields the following expression for local shear stress as a function of distance from the propellant surface and local cross-flow velocity:

\[ \tau = \frac{\rho \tau_f}{\rho_s} \left( C_f/2 \right) \] (33)

At any rate, application of Eqs. 29-34 permits calculation of local shear stress, \( \tau \) as a function of distance from the propellant surface \( y \) and local cross-flow velocity \( u \) for a given set of free-stream conditions, mass injection rate, and temperature field, \( \rho = \rho_0, u(y) \). An eddy viscosity approach is used to relate the local shear stress to the local cross-flow velocity gradient via:

\[ \tau = (u - \rho e) \frac{du}{dy} \] (35)

With specification of an expression for \( \varepsilon \) as a function of \( y \) and \( du/dy \) (discussed below), and use of:

\[ \varepsilon = \frac{P(MO)/RT}{u} \] (36)

\[ u = kT \] (37)

\[ \tau = \frac{T_f - T_s}{s} \frac{(s_f - s)Y_s}{RX \rho_9 \sin \theta} \] (38)

(the latter equation resulting from assumption of a linear temperature profile from the surface to the end of the diffusion flame), Eq. 35 may be combined with the \( \tau = \rho_3 (u_3 y) \) relationship obtained from Eqs. 29-34 to yield a first order differential equation for local cross-flow velocity. With use of \( u = 0 \) at \( y = 0 \), this is numerically integrated from the wall to yield \( u(y), \varepsilon(y), \rho(y), \) and \( u(y) \). In addition, with use of \( v(y) = \frac{\rho_3 y}{ho} \), \( v(y) \) is obtained and the shape of streamlines emanating from the surface is used to calculate a correction to the effective diffusion flame bending angle, \( \theta \), allowing for the fact that the bent flame is curved rather than straight, as assumed in the earlier version of the erosive burning package. These results are used to calculate

\[ \lambda_{eff} = \frac{\lambda_{eff}^2 \rho_d^2 \rho_d^2}{\lambda_{eff}^2 \rho_d^2} + 10 - c = \rho_3 (y) \] (39)

That is, the ratio of transport total properties to laminar properties is calculated as a function of distance from the surface. Average total transport property values between appropriate zones are then calculated and substituted for the laminar values in the diffusional mixing equations and the heat feedback equations in the original model, revised burn rates and flame distances are calculated, and the procedure is repeated until convergence is achieved. As might be expected, this looping procedure is considerably more complex in the case of multimodal propellants than for unimodal propellants since solution of the individual sub-propellant cases becomes interactive in the case of crossflow. This interaction occurs because there is only one boundary layer for the overall propellant (that is, one boundary layer profile for each subpropellant) with the boundary layer details being controlled by the average transpiration velocity, flame height, surface temperature, etc., for the overall propellant rather than by the individual values of these parameters for each subpropellant.

Several options for closure of the boundary layer analysis through use of an eddy viscosity equation were built into the program: all entailed use of a Prandtl mixing-length type expression.

The most comprehensive of these was a modified form of an empirical relation developed by Kays and Moffat \((11)\) which includes the effects of blowing and axial pressure gradient but does not include the effects of roughness. The modifications added by this author were an attempt to include the effects of roughness using approaches suggested by the works of van Driest \((15)\) and Cebechi and Chang \((16)\). The resulting expression is:

\[ c = 0.168 (y + y_0) \frac{du}{dy} \left[ 1.0 - \exp \left\{ -2.6 \left( y + y_0 \right) \right\} \right] \] (40)

\[ c = 0.168 (y + y_0) \frac{du}{dy} \frac{Ku}{v > 65} \] (40)

where:

\[ ky = 0.9 \left( \frac{u_k}{v} - \exp \left[ \frac{-1}{\sigma} \right] \right) \] (41)

\[ ky = 0 \text{ for } v \leq 4.535 \] (42)

The second exponential in Eq. 40 is included to force the damping function (major brackets) to go to unity as the roughness Reynolds Number \( Ku/v \) approaches 65 (full roughness), consistent with the van Driest \((15)\) approach. The \( ky \) term reflects a profile displacement due to roughness as suggested by Cebechi and Chang \((16)\). Other options considered included use of the van Driest expression without blowing or pressure gradient effects, use of the above expression with \( ky \) set equal to zero for all roughness values, and use of an expression with no damping (with or without a roughness \( ky \) factor). The expression which thus far seems to give the best results is the no-damping, no-roughness expression:

\[ c = 0.168 (y + y_0) \frac{du}{dy} \] (43)

though it must be admitted that this is not the most pleasing on physical grounds.

As mentioned earlier, depending on the \( C_f/C_{f0} \) relationship used there are cases (high blowing parameter ones) where attempts to integrate the shear stress equation out from the surface results in the local shear stress going negative; this is interpreted as representing some type of boundary layer blowoff. In this case, it is assumed that the velocity profile assumes the cosine law shape (inviscid no-wall-slip flow) measured by Yamada and Goto \((47)\) among others, and this profile is then differentiated and the result substituted into Eq. 43 to yield the eddy viscosity distribution, without
The same constants for the fourth propellant resulted in a more physically correct model. The predictions shown in Figure 3 gave excellent agreement with the no-crossflow burn rate data for the unimodal and multimodal propellants (with the result that a set of constants which gives good agreement between theory and data for the 1667*K formulations tends to result in underprediction of burn rate for the hotter formulation. It was this result that led to development of Variants IIIA, IIIB, and IIIC, in which more emphasis was placed on insuring that overall formulation flame temperature would have more direct influence on the predicted burning rate.

Variant IIIB was found to give unsatisfactory results for all values of the fuel-assignment parameter (XXA) examined and was consequently dropped. The search for an optimum value of XNA was limited to values between 0 and -1: it may be that a more negative value would result in improvement of agreement between theory and data, but it seemed more worthwhile to pursue Variants IIIA and IIIC since they seemed more attractive on physical grounds (particularly IIIC) and required fitting of one less empirical constant.

Predicted and experimental burn rate versus pressure results for the four unimodal formulations in the absence of crossflow are presented for Variants IIIA, IIIC, and IV in Figures 2, 3, and 4, respectively. As may be seen, with optimization of the three free constants (IIIB) highly desirable for the three variants, as might be expected) all three variants permit excellent prediction of the burning rate versus pressure characteristics of the four formulations, Variant IIIIA giving the best agreement of theory with data. Since Variant IV did not give appreciably worse results than the other two variants and was considerably simpler to extend to treatment of multimodal oxidizer formulations and to crossflow cases using the erosive burning package described in the previous section, it was selected for first extension to those cases.

Multimodal Oxidizer Propellants, No Crossflow

The extension of Variant IV of the Generation 2 model to handle multimodal oxidizer cases was described in the preceding section. Results of use of this extended model to predict no-crossflow burn rate versus pressure behavior for the two multimodal oxidizer formulations listed in Table II are presented in Figure 5. It should be noted that the values of $K_{OP}$, $K_{OF}$, and $B_{sub}$ selected during analysis of the unimodal oxidizer formulations are not changed: that is, they are no longer free constants. The predictions shown in Figure 5 were made with the fuel-assignment constant (XXP) set equal to 3 (resulting in equal stoichiometry subpropellants).
As may be seen, agreement between theory and data is excellent except at the high pressure end of data for the 90/200 micron formulation (5565). The two highest pressure data points for this formulation appear to fall off from the trend while the predicted rates continue to climb. The reason for this behavior is not clear. Limited calculations using lower values of XEXP (corresponding to the small oxidizer size subpropellant being more fuel-rich than the large oxidizer size subpropellant) yielded worse agreement with data.

**Erosive Burning Predictions Using Only Flame-Bending**

As discussed earlier, all of the model variants examined originally contained an erosive burning package based on the assumption that the sole mechanism causing burning rate increase with crossflow is the bending over of columnar diffusion flames by that flow. (This package is described in detail for Variant I in Ref. 5.) For all variants, with free constants optimized from matching no-crossflow data as described earlier, this assumption led to the underprediction of crossflow effects for all formulations at all pressures and crossflow velocities. An example of this underprediction is shown in Figure 6, where predictions made using Variant IV with the original erosive burning package are compared with data for Formulation 4525 (73/27 AP/HTPB, 20 micron AP). Based on these results, the erosive burning portion of the Generation 2 model was revised as described in the previous section to allow consideration of augmentation of gas transport properties by crossflow-induced turbulence as well as flame bending.

**Erosive Burning Data Comparison With Revised Model Predictions**

Several different eddy viscosity models and several equations for extrapolation of skin friction data to high blowing ratio conditions were built into the revised Variant IV model, as discussed earlier. Studies to date indicate that the erosive burning data for the formulations listed in Table II are best predicted using the no-damping, no-roughness eddy viscosity expression (Eq. 43) and the first of the four Cf/Cfo expressions (Eq. 32a), but a firm conclusion regarding the most suitable expressions has not yet been made. (As indicated, a major difficulty with this analysis is that it involves making boundary layer predictions in a blowing-ratio regime which has not been studied, and extrapolation of turbulent flow field data is extremely risky.) Theoretical predictions and data for the six formulations tested to date are presented in Figures 7 - 12. As may be seen, the agreement between theory and data for five of the six formulations is quite encouraging. With Formulation 5565 (the 82/18 AP/HTPB bimodal formulation with 90 and 200 micron ammonium perchlorate) however, the model predicts considerably more sensitivity of burning rate to crossflow than actually observed. Use of Eqn. 32d for calculation of Cf/Cfo results in considerable improvement of agreement between theory and data for this formulation, but only at the expense of worsening agreement between theory and data for the other five formulations. Thus far, no combination of eddy viscosity/ Cf/Cfo expressions considered has resulted in improvement of the predictions for the "problem" formulation without simultaneously degrading the agreement between theory and experiment for the other formulations.

Considerable thought has been devoted to this problem, resulting in definition of an interesting dilemma. Formulation 4525 (73/27 AP/HTPB, 1667K flame temperature, 20 micron oxidizer) and Formulation 5565 (82/18 AP/HTPB, 2755K flame temperature, bimodal mix of 90 and 200 micron oxidizer) were tailored to give nearly identical burn rate versus pressure characteristics in the absence of crossflow. This near equality of burning rates resulted from cancellation of a considerably higher temperature driving force (flame temperature) for the latter formulation by a lower flame distance associated with the smaller oxidizer formulation. That is, in a no-crossflow situation the diffusion flame zone stretches considerably further from the surface for the 5565 formulation, offsetting the effect of higher flame temperature on burn rate. Thus, it would appear that the heat release regions, being much further out into the higher turbulence (and stronger flame-bending) region of the boundary layer for the 5565 formulation should be much more affected by crossflow for this formulation than for Formulation 4525, and thus the burning rate of 5565 should be much more sensitive to crossflow than that of 4525. Indeed, this is what is predicted by the model and is what it seems to this author must be predicted by any model based on either diffusion-flame bending or turbulence augmentation of transport properties. However, comparison of the data in Figures 8 and 12 reveals that the erosive burning characteristics of these two formulations are essentially identical. This appears to be a fundamental problem for which this author does not currently have an explanation.

**Summary**

Several variants of a model for the non-erosive burning of unimodal oxidizer composite propellants have been developed. These variants have been tested, with optimization of three "free" constants against no-crossflow burning rate data for a family of four AP/HTPB propellants experimentally studied at Atlantic Research. Three variants, including two which treat the incrementl regression of the burning front through an oxidizer crystal and one in which an average-intersection concept is employed, have been found to predict the data quite well. The average-intersection variant was extended to handle crossflows and multimodal oxidizer formulations. This extended model was found to give excellent agreement with no crossflow burning rate data for two additional formulations containing bimodal oxidizer. In the initial development of the erosive burning aspect of the model, columnar diffusion flame bending was assumed to be the only mechanism leading to burn rate augmentation by crossflows. This assumption led to severe underprediction of erosive burning effects, and a flow profile analysis for prediction of turbulence augmentation of transport properties as well as flame-bending was subsequently built into the model. This revised model is found to give good agreement with burning data for five of the six formulations studied, but gives predicted rates higher than observed for the sixth formulation. It is felt that this problem results from an inability to accurately predict turbulence profiles at high blowing ratios (transpiration velocity/crossflow velocity) in comparison with the fact that the formulation contains very large oxidizer particles, making its predicted burning rate quite sensitive to the boundary layer details.
### Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>AFU</td>
<td>fuel surface area associated with APOX</td>
</tr>
<tr>
<td>APOX</td>
<td>planar projection or exposed oxidizer particle surface area</td>
</tr>
<tr>
<td>ASOX</td>
<td>total curved oxidizer exposed surface area</td>
</tr>
<tr>
<td>$B_{sub}$</td>
<td>pre-experimental for subsurface reaction rate equation</td>
</tr>
<tr>
<td>$b$</td>
<td>blowing parameter, defined by Eq. 31.</td>
</tr>
<tr>
<td>$C_f$</td>
<td>skin friction coefficient, including transpiration effects</td>
</tr>
<tr>
<td>$C_{f0}$</td>
<td>no-blowing skin friction coefficient</td>
</tr>
<tr>
<td>$C_p$</td>
<td>solid oxidizer heat capacity</td>
</tr>
<tr>
<td>$C_{pox}$</td>
<td>oxidizer particle diameter</td>
</tr>
<tr>
<td>$D_0$</td>
<td>distance of center of oxidizer crystal surface from initial oxidizer peak</td>
</tr>
<tr>
<td>$D_{POX}$</td>
<td>diamater corresponding to APOX surface projection propellant surface</td>
</tr>
<tr>
<td>$D_{eff}$</td>
<td>effective total gas diffusivity (molecular plus turbulent)</td>
</tr>
<tr>
<td>$E_{ACT,OF}$</td>
<td>activation energy for fuel-oxidizer gas reaction</td>
</tr>
<tr>
<td>$E_{ACT,AP}$</td>
<td>activation energy for monopropellant oxidizer gas reaction</td>
</tr>
<tr>
<td>$E_{sub}$</td>
<td>activation energy for subsurface reaction and fuel gas streams</td>
</tr>
<tr>
<td>FHPD</td>
<td>distance required for mixing of oxidizer and fuel gas streams</td>
</tr>
<tr>
<td>h</td>
<td>channel half-height</td>
</tr>
<tr>
<td>k</td>
<td>constant defined by Eq. 34</td>
</tr>
<tr>
<td>$K_{AP}$</td>
<td>constant in expression for oxidizer monopropellant reaction distance</td>
</tr>
<tr>
<td>$K_{OF}$</td>
<td>constant in expression for OF gas reaction distance</td>
</tr>
<tr>
<td>$L_{AP}$</td>
<td>oxidizer monopropellant gas reaction distance</td>
</tr>
<tr>
<td>$L_{ox}$</td>
<td>oxidizer/fuel gas reaction distance</td>
</tr>
<tr>
<td>$L_{crossflow}$</td>
<td>cross flow Nusselt number (mean)</td>
</tr>
<tr>
<td>MW</td>
<td>molecular wight</td>
</tr>
<tr>
<td>$N_{INJ}$</td>
<td>surface blowing mass flux (burning mass flux based on planar area)</td>
</tr>
<tr>
<td>$n_{fuel}$</td>
<td>oxidizer mass flux, based on planar surface projection</td>
</tr>
<tr>
<td>$n_P$</td>
<td>mass flux of propellant (or subpropellant) based on planar surface area</td>
</tr>
<tr>
<td>n</td>
<td>global gas-phase reaction order</td>
</tr>
<tr>
<td>P</td>
<td>pressure</td>
</tr>
<tr>
<td>$R_g$</td>
<td>gas law constant</td>
</tr>
<tr>
<td>Re</td>
<td>Reynolds Number based on channel hydraulic diameter</td>
</tr>
<tr>
<td>$R_{av}$</td>
<td>average linear regression rate of propellant</td>
</tr>
<tr>
<td>$R_{fuel}$</td>
<td>linear regression rate of fuel surface normal to its curved surface temperature</td>
</tr>
<tr>
<td>$R_{ox}$</td>
<td>linear regression rate of oxidizer surface temperature</td>
</tr>
<tr>
<td>$T$</td>
<td>temperature at location of monopropellant oxidizer flame</td>
</tr>
<tr>
<td>$T_{AP}$</td>
<td>temperature of oxidizer melting temperature</td>
</tr>
<tr>
<td>$T_{bulk}$</td>
<td>propellant bulk (initial) temperature</td>
</tr>
<tr>
<td>$T_melt$</td>
<td>surface temperature</td>
</tr>
<tr>
<td>$T_{ub}$</td>
<td>time for fuel regression plane to move from one increment to the next</td>
</tr>
<tr>
<td>$u(y)$</td>
<td>crossflow velocity at distance y from the surface</td>
</tr>
<tr>
<td>$u_{crossflow}$</td>
<td>mean crossflow velocity</td>
</tr>
<tr>
<td>$U_{fs}$</td>
<td>mainstream crossflow velocity</td>
</tr>
<tr>
<td>$U_f$</td>
<td>friction velocity, $U_{fs}\sqrt{C_f/2}$</td>
</tr>
<tr>
<td>$k$</td>
<td>defined by Eq. 15</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>mass fraction oxidizer reacting at or below propellant surface</td>
</tr>
<tr>
<td>$\beta_{propellant}$</td>
<td>mass fraction oxidizer in overall propellant</td>
</tr>
<tr>
<td>$\rho_{fuel}$</td>
<td>fuel (binder) density</td>
</tr>
<tr>
<td>$\rho$</td>
<td>gas density</td>
</tr>
<tr>
<td>$\rho_{fs}$</td>
<td>mainstream gas density</td>
</tr>
<tr>
<td>$\mu$</td>
<td>viscosity (laminar)</td>
</tr>
<tr>
<td>$\tau(y)$</td>
<td>shear stress at distance y from the propellant surface wall shear stress</td>
</tr>
<tr>
<td>$\nu$</td>
<td>kinematic viscosity, $\mu/\rho$</td>
</tr>
</tbody>
</table>

### References


Table I. Unimodal Oxidizer (No Cross Flow) Generation 2 Model Variants Examined

I. ORIGINAL GENERATION 2 MODEL, DESCRIBED IN DETAIL IN REFERENCE 5. UNIFORM DISTRIBUTION OF O/F FLAME HEAT RELEASE BETWEEN $X = LRX$ AND $X = LRX + FH90$. LAP INDEPENDENT OF LOCAL TEMPERATURE. STEP THROUGH VARIOUS INTERSECTIONS OF OXIDIZER AND FUEL, WITH 3 WAYS OF AVERAGING BURN RATE EMPLOYED.

II. SAME AS I, EXCEPT FOR USE OF AN AVERAGE FUEL-OXIDIZER INTERSECTION CONCEPT.

III. MODIFICATION OF I. ALLOWANCE FOR DEPENDENCE OF LAP ON LOCAL TEMPERATURE. ALTERED DEPENDENCY OF LRX ON $T_{flame}$. SUBSURFACE HEAT RELEASE CALCULATION MODIFIED TO ALLOW FOR REACTANT DEPLETION. WEIGHTING OF DISTRIBUTION OF O/F FLAME HEAT RELEASE BETWEEN TOP AND BOTTOM OF CONICAL FLAME CHANGED TO BE MORE CONSISTENT WITH DETAILED MIXING PROFILES CALCULATED VIA BURKE-SCHUMANN ANALYSIS.

IV. SAME AS III, EXCEPT FOR USE OF AN AVERAGE FUEL-OXIDIZER INTERSECTION CONCEPT.

V. SAME AS III, EXCEPT FOR ALLOWANCE OF DIFFERENT SURFACE TEMPERATURES FOR BINDER AND OXIDIZER. DIFFUSION FLAME HEIGHTS RELATIVE TO AP SURFACE ADJUSTED TO ALLOW FOR ITS PROJECTION OR DEPRESSION RELATIVE TO BINDER CONTINUUM SURFACE.

VI. SAME AS V, EXCEPT NO ADJUSTMENT OF DIFFUSION FLAME HEIGHTS (WRINKLED FLAME).

III.B. SAME AS III, EXCEPT THAT FLAME TEMPERATURE IS SET EQUAL TO FLAME TEMPERATURE ASSOCIATED WITH OVERALL COMPOSITION AT ALL INTERSECTIONS.

III.C. SAME AS III, EXCEPT O/F RATIO IS FORCED TO BE CONSTANT (AT OVERALL PROPELLANT O/F) AT EACH INTERSECTION BY ADJUSTMENT OF THE ASSOCIATED FUEL AREA AS THE OXIDIZER-SURFACE INTERSECTIONAL AREA CHANGES.

Table II. Propellants Used in Model Checkout.

<table>
<thead>
<tr>
<th>FORMULATION DESIGNATION</th>
<th>AP/HTPB RATIO</th>
<th>OXIDIZER PARTICLE SIZE (S), MICRONS</th>
<th>THEORETICAL FLAME TEMPERATURE, °K</th>
</tr>
</thead>
<tbody>
<tr>
<td>4525</td>
<td>73/27</td>
<td>20</td>
<td>1667</td>
</tr>
<tr>
<td>4685</td>
<td>73/27</td>
<td>5</td>
<td>1667</td>
</tr>
<tr>
<td>5051</td>
<td>73/27</td>
<td>200</td>
<td>1667</td>
</tr>
<tr>
<td>5542</td>
<td>77/23</td>
<td>20</td>
<td>2065</td>
</tr>
<tr>
<td>5565</td>
<td>82/18</td>
<td>[13.65% 90]</td>
<td>2575</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[60.35% 200]</td>
<td></td>
</tr>
<tr>
<td>5555</td>
<td>82/18</td>
<td>[41% 1]</td>
<td>2575</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[41% 7]</td>
<td></td>
</tr>
</tbody>
</table>

Figure 1. Schematic of Burning Composite Propellant, With and Without Cross Flow
Figure 6. Comparison of Erosive Burning Data with Theoretical Predictions Made Assuming Flame-Bending to be the Only Mechanism Causing Burn Rate Augmentation

Figure 7. Erosive Burning Data and Predictions – 73/27 AP/HTPB, 5µAP

Figure 8. Erosive Burning Data and Predictions – 73/27 AP/HTPB, 20µAP

Figure 9. Erosive Burning Data and Predictions – 73/27 AP/HTPB, 200µAP
Figure 10. Erosive Burning Data and Predictions - 77/23
AP/HTPB, 20μAP

Figure 11. Erosive Burning Data and Predictions - 82/18
AP/HTPB, 41% 1μAP, 41% 7μAP

Figure 12. Erosive Burning Data and Predictions - 82/18
AP/HTPB, 13.65% 90μAP, 68.35% 200μAP