# Effect of Geometry on Ignition of a Reactive Solid: **Square Corner**

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A numerical study has been initiated to investigate quantitatively the effects of geometry on the ignition characteristics of a reactive solid exposed to interrupted heating rates. The initial geometry selected was a semi-infinite square corner. Reactant depletion was included. Critical ignition conditions were determined for a wide range of physiochemical parameters by numerical integration of the equations via forward finite difference techniques. Geometry and parameter effects were delineated by performing detailed comparisons to existing one-dimensional results, indicating that 1) the ignition delay was reduced by a factor of 2.5 to 3.4 depending upon particular parameter values, 2) critical ignition temperatures were slightly higher for the two-dimensional case, 3) reactant depletion had a much more dominant effect, and 4) an empirical formula describing the critical ignition delay time as a function of system parameters was developed and reduced to the same form as the one-dimensional case except for a differing constant of proportionality.

### Nomenclature

=  $Q\nu kT_i/q^2$ , dimensionless parameter  $= Q/\rho cT_i$ , dimensionless parameter = specific heat, kJ/kg K C E E' = constant of proportionality, see Eq. (7) = activation energy, MJ/kmol  $= E/RT_i$ , dimensionless parameter k = thermal conductivity,  $\overline{W}/m K$ = incident heat flux, W/m<sup>2</sup>

Q R= heat of reaction, MJ/m<sup>3</sup> = universal gas constant, 8.36 kJ/kmol K

= time, s

= temperature, K = space coordinates, m

= fraction of reactant consumed  $= qy/kT_i$ , dimensionless distance  $= T/T_i$ , dimensionless temperature = pre-exponential factor, s

ξ  $= qx/kT_i$ , dimensionless distance

= density,  $kg/m^3$ ρ

=  $q^2 t/k\rho cT_i^2$ , dimensionless time

# Subscripts

= critical value, referring to value at end cof critical heating period

= initial

= value referring to duration of heating = critical value, computed for inert material

# Introduction

COMMONLY accepted fact is that in the ignition of solid materials roughness—i.e., the presence of sharp edges—can increase the rapidity of ignition. Frequently one speaks of "rough is better than smooth" and "split wood burns better" when the problem is the lighting of a campfire.

The "fuzzsticks" from the Boy Scout manual may come to mind in this connection. On a more technical plane, the ignition delay of material of interest to solid propellant specialists may be in the range of a few milliseconds or less after exposure to some ignition stimulus. The thermal wave penetration into the material during this time, for typical propellants, can range from 20 to 200 µm. In many cases this is of the same order of size as the surface roughness of the propellant, either by the structure of the propellant itself or by the physical deformations produced during the manufacture of the propellant grains. Therefore, on the ignition time scale, the surface is not strictly one-dimensional. Virtually all theoretical ignition studies concerning solid propellants are one-dimensional. What, therefore, is the effect of this multidimensionality on the ignition delay of a solid propellant, particularly when sharp edges are present? This paper addresses this question for the particular case of a homogeneous reactive solid exposed to a constant applied heat flux when the edge is formed by a right-angled corner.

An earlier study<sup>1</sup> showed that a homogenous reactive solid whose geometry forced a convergence of the heat flow lines from the heated surface could greatly accelerate the ignition process. This was shown for a cylindrical geometry having a constant heat flux radially applied. While this geometry is mathematically one-dimensional and hence analytically solvable by standard methods, convergent heat flow lines were present. When the cylinder had a sufficiently small radius (1 mm or less), the ignition delay was significantly shortened.

Another investigation<sup>2</sup> briefly discussed the ignition process of a homogeneous reactive solid having a right-angled corner and a single set of property values. Chemical reaction was assumed to occur only at the surfaces exposed to a constant applied heat flux. Numerical predictions compared favorably to experimental results, both indicating a substantial reduction in the ignition time for the two-dimensional case vs the well-known one-dimensional geometry.

As a cylinder did not adequately represent a sharp corner and the work by Baer and Ryan<sup>2</sup> was limited to a single set of physiochemical properties, an extensive numerical study concerned with the effect of a corner geometry on the ignition process of a homogeneous reactive solid was initiated.

## Model Description

To learn the effects that a sharp corner might induce on the ignition process of a solid propellant, the right angle formed

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by considering the first quadrant in a Cartesian coordinate system was the geometry selected. For mathematical convenience and to allow direct comparison with well-known analytical and numerical results,<sup>3,4</sup> a homogeneous, opaque reactive solid was selected to represent a solid propellant. In addition, the physical properties of the solid were assumed to be constant, independent of the temperature or the extent of decomposition, and the exothermic reaction in the solid phase was represented by a single-step Arrhenius bulk reaction rate. External gas phase reactions were ignored entirely, and, starting at zero time, a constant heat flux was applied normally to the surfaces bounded by the lines (0, y > 0) and (x > 0, 0). The applied flux remained constant for some specified time after which the flux was set to zero and the exposed surfaces were thermally insulated. Reactant consumption was included, but reaction products were assumed to remain solid and maintain identical property values. Boundary surfaces were assumed to remain stationary. Figure 1 shows a schematic of the physical model.

Dimensionless variables, including an additional space variable, are defined as in Refs. 3 and 4 and listed in the Nomenclature. The present model is completely specified by the following equations and initial boundary conditions as

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial \xi^2} + \frac{\partial^2 \theta}{\partial \eta^2} + A(1 - \epsilon) \exp^{-E'/\theta}$$
 (1)

$$\frac{\partial \epsilon}{\partial \tau} = \left(\frac{A}{B}\right) (1 - \epsilon) \exp^{-E'/\theta} \tag{2}$$

$$\theta(\xi, \eta, 0) = 1, \quad \epsilon(\xi, \eta, 0) = 0 \quad (\xi > 0, \eta > 0) \quad (3a)$$

$$\frac{\partial \theta}{\partial \xi}(\infty, \eta, \tau) = \frac{\partial \theta}{\partial \eta}(\xi, \infty, \tau) = 0$$
 (3b)

$$\frac{\partial \theta}{\partial \xi}(0, \eta, \tau) = \frac{\partial \theta}{\partial \eta}(\xi, 0, \tau) = -1 \quad 0 < \tau < \tau_h \quad (3c)$$

$$= 0 \tau > \tau_h (3d)$$

Parameter A is the ratio of chemical energy to external heating rates, and B, called the dimensionless heat release parameter, is the ratio of chemical energy available in the solid to the initial sensible energy. A and E' together fully specify the characteristics of the heat production term in Eq. (1).

## **Qualitative Model Behavior**

Equations (1-3), containing nonlinear Arrhenius and concentration terms, represent a specific form of the general transient heat conduction equation, including a bulk heat generation term. The attainment of ignition can be described as the applied flux driving a thermal wave in the corner geometry which diffuses continuously into the interior. Simultaneously with the diffusion process the material undergoes an

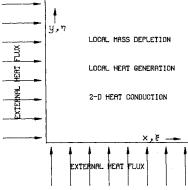


Fig. 1 Schematic of the physical model.

exothermic bulk reaction, and the amount of heat liberated locally follows the assumed Arrhenius reaction rate.

The heating process of the reactive solid initially follows that of an inert material; the initial corner temperature history is indistinguisable from that of an inert material of the same geometry. Later, as the local heat generation rate becomes of the same order as the applied flux, the corner temperature increases faster, possibly resulting in successful ignition. However, reactant consumption interacts with the self-heating effect and tends to diminish the rate of the corner temperature rise.

As done by Bradley<sup>4</sup> for the one-dimensional analog of the present study, the applied heating is suddenly removed and exposed surfaces are taken to be insulated. The critical ignition delay for the interrupted heating mode  $\tau_c$  is presently defined as the shortest heating time such that after the longest possible induction period a runaway in temperature occurs in the corner region. The sensitivity of the temperature field behavior to the time of the flux removal in the present investigation is greater than that reported by Bradley<sup>4</sup> and reduces the length of the induction period. Whereas Bradley<sup>4</sup> reportedly achieved induction periods ranging from 0.2 to  $5\tau_c$ , the increased temperature sensitivity in the current study limited the length of the induction period to a maximum of  $0.9\tau_c$ . Higher E' values generally resulted in shortened postheating periods for the two-dimensional geometry. Critical conditions for the continuous heating case were determined at the onset of a rapid rise in the corner temperature.

## **Solution Technique**

The discretized dimensionless equations were integrated numerically via forward finite differences, using special care with respect to spatial and time steps to ensure good convergence of the solutions obtained. The solution domain was subdivided into uniform segments  $\Delta \xi$  by  $\Delta \eta$  with a node located at the centroid of each segment. The "nodal value" represents the temperature or fraction reacted for that segment. The analytical solution of the two-dimensional heat conduction problem (A = 0) was used to establish a starting temperature field to lessen overall computation time. Transition to the reactive finite-difference equations took place based on the highest temperature node when the contribution of the  $A(1-\epsilon) \cdot \exp(-E'/\theta)$  term to the change in internal energy for that node was between 0.4 and 1%. This criterion compared well with a "linearity" criterion defined by Hicks,5 which was also evaluated at the highest temperature node and is discussed further in Ref. 6. The equations were solved using the same parameter range as Bradley,4 namely

$$A = 1.5 \times 10^8$$
 to  $1.5 \times 10^{29}$   
 $B = 0.9$  and 4.5  
 $E' = 331/3, 50, 662/3, 831/3, and 100$ 

These selections represented combinations of the following

$$Q\nu = 4.18 \times 10^7$$
 to  $4.18 \times 10^{30}$  MJ/m<sup>3</sup>

$$Q = 669 \text{ and } 3344 \text{ MJ/m}^3 \text{ (approximately 0.1 and 0.5 of the total heat of combustion of solid propellant)}$$

$$E = 83.6 \text{ to } 250.8 \text{ MJ/kmol}$$

$$q = 418 \text{ to } 41.8 \times 10^6 \text{ W/m}^2$$

$$\rho = 1600 \text{ kg/m}^3$$

c = 1.547 kJ/kg K

values of physical constants:

k = 0.209 W/m K

 $T_i = 300 \text{ K}$ 

Results consisted of critical values of  $\theta$ ,  $\epsilon$  and  $\tau$  as a function of parameters A, B, and E'. They indicated that the maximum temperature and fraction reacted always occurred at the extreme corner node, which is not a particularly surprising result. Critical conditions and the successful attainment of ignition were therefore based on the behavior of this node. When  $\epsilon$  values of about .60 existed close to the spatial point of ignition, a true thermal runaway did not occur in the present model, primarily because of the dampening effect that the diminished reactant concentration had on the chemical heat production term. Smaller critical  $\epsilon$  values did not affect the ignition behavior to such a drastic extent.

Finally, the boundary condition of Eq. (3b) was imposed not at infinity but after a finite number of grid steps (40) in each coordinate direction. This was necessary to obtain reasonable computation (CPU) times on the DEC-2060 computer used in the integrations. The error induced by this approximation was extensively checked<sup>6</sup> by several numerical runs without this limitation over a representative range of parameter values. We found that this approximation affected critical values by less than 0.05%.

## Results

Results of the integrations will be presented in the same fashion used by Bradley<sup>4</sup> to allow the direct comparison of two-dimensional and one-dimensional cases. Both continuous and interrupted heating modes were considered, but results are presented in terms of the interrupted heating mode unless indicated otherwise. Figure 2 shows the attainment of ignition for both continuous and interrupted heating for a common set of parameters. Ignition delays computed for the continuous heating case exceed the interrupted heating data by 0.5 to 2.5%. At low  $\tau_c$  values the difference in ignition delay for the two modes of heating increases to 8 or 9%, which can be attributed to the onset of homogeneous explosion phenomena.<sup>7</sup>

Figures 3 and 4 show the relationships among the critical values of  $\tau$ ,  $\epsilon$ , and  $\theta$  for parameters A, B, and E'. Figure 3 corresponds to B = 4.5 and Fig. 4 to B = 0.9. Direct comparison indicates that identical E' curves differ only slightly. Hence parameter B has little effect on ignition time if ignition takes place and does not strongly affect the ignition temperature  $\theta_c$ . The midsections of E' curves are practically straight, with slope 8/E' permitting an empirical expression relating parameters A and E' to the ignition delay  $\tau_c$ . Crossdrawn in Figs. 3 and 4 are the critical fraction reacted and ignition temperature as a result of the integrations. The  $\epsilon_c$  curves become more closely spaced with increasing  $\epsilon_c$  values, illustrating the effect of the  $(1 - \epsilon)$  term. Progressively more reactant is needed to supply the heat generation required for thermal runaway. Upper critical limits exist for both  $\epsilon_c$  and  $\theta_c$ beyond which successful ignition does not occur. Both phenomena are related to the near total depletion of reactants in

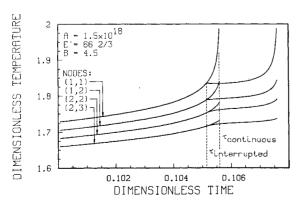


Fig. 2 Dimensionless corner temperature profiles showing the effect of the mode of heating on the ignition time for a selected set of parameter values.

the corner region prior to the attainment of a runaway in temperature.

Figure 5 shows the dependence of the critical corner temperature on parameters A and E' for both B values. Clearly the ignition temperature is not constant but increases along a given E' curve with higher heating rates. Higher heating rates form steeper thermal gradients, thinner heated layers, and therefore more rapid cooling after flux termination.

Figure 6 shows the curve of ignition temperature  $\theta_c$  vs ignition delay  $\tau_c$  for all possible parameter combinations. Excluding data points having a high  $\epsilon_c$  value, this universal curve is represented to 4% accuracy by

$$\theta_c = 1 + 2.572(\tau_c)^{1/2} \tag{4}$$

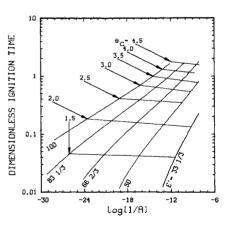
while the corresponding equation for the inert heating case is given by

$$\theta_1 = 1 + 4(\tau_c/\pi)^{1/2} \tag{5}$$

Equations 4 and 5 indicate that

$$(\theta_c - 1)/(\theta_l - 1) = 1.14$$
 (6)

which implies that for successful ignition to occur, the critical corner temperature for a reactive solid must exceed its inert counterpart by 14%. Similarly, a ratio of reactive to inert heating times may be developed, producing the same temperature level which yields a representative value of 0.77 for the present geometry. This means that the time required to reach any ignition temperature for a reactive solid is roughly equal to 77% of the inert heating time to achieve that same temperature level, provided that total reactant consumption has not occurred.



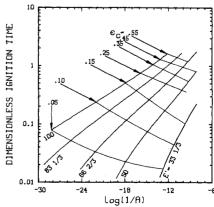


Fig. 3 Numerical results for B=4.5 showing dimensionless ignition delay  $\tau_c$  vs  $\log(1/A)$ ; critical  $\theta_c$  and  $\epsilon_c$  curves included.

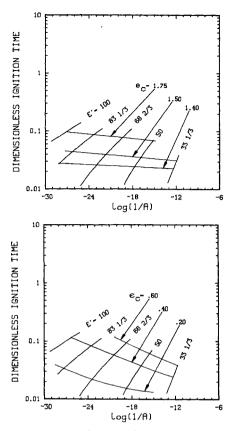


Fig. 4 Numerical results for B=0.9 showing dimensionless ignition delay  $\tau_c$  vs  $\log(1/A)$ ; critical  $\theta_c$  and  $\epsilon_c$  curves included.

Figure 7 shows the dependence of the critical heating time  $t_c$  (proportional to the quantity  $A\tau_c$ ) on the applied heat flux q (proportional to the quantity  $1/\sqrt{A}$ ). Experimental ignition results are typically displayed in this fashion.

# Comparison with the One-Dimensional Case

As previously mentioned, Bradley<sup>4</sup> has presented the most complete study for the one-dimensional case of the present problem, and is therefore the major source for comparison.

The definition of ignition was slightly modified from Bradley's<sup>4</sup> version since it was not numerically achievable in the present case. Either a rapid ignition or a steady temperature drop, leading to extinction, occurred shortly after flux termination, contrary to the extensive induction period reported by Bradley.<sup>4</sup> This is an interesting and significant difference in behavior between the one- and two-dimensional problems. Figures 8 and 9 show typical corner temperature behavior during the induction period, illustrating a short postheating period prior to thermal runaway and extreme sensitivity to duration of heating. A variation in heating time of 10<sup>-5</sup> to 10<sup>-4</sup> in dimensionless time units generally meant the difference between ignition and extinction.

Comparison of present numerical results (Figs. 3 and 4) to Bradley's<sup>4</sup> (Fig. 3) reveals a similar overall appearance except for the downward shift of the present E' curves with respect to the vertical coordinate. Figure 10 shows the ratio of ignition times of semi-infinite slabs to semi-infinite 90 deg corners as a function of parameter A [one-dimensional data developed from Bradley's Eq.  $(17)^4$ ]. Three distinctive physical phenomena can be observed here. First, the vertical positioning of E' curves is explained by considering the nature of the heating process for different E' values. A ratio of heating times of 4.0 can easily be derived for the respective one- and two-dimensional inert cases. Reactive curves at high E' value approach

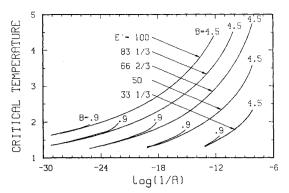


Fig. 5 Dimensionless critical corner temperature  $\theta_c$  vs  $\log(1/A)$  for constant activation energy E' and B equal to 4.5 and 0.9.

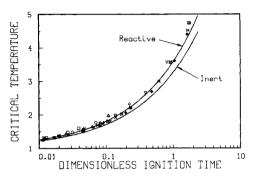


Fig. 6 Dimensionless critical corner temperature  $\theta_c$  vs dimensionless ignition delay  $\tau_c$  for interrupted heating. Linear corner temperature curve included.

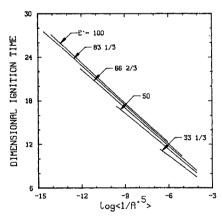


Fig. 7 Effect of flux level on critical heating time.

this inert heating ratio better as a result of a longer portion of the heating being characterized by the heating of an inert solid. Second, the E' curves appear to converge as parameter A decreases to zero, which implies infinite heating rates. Physically the chemical reaction time becomes very small and independent of activation energy parameter E'. Finally, the ignition times ratio reduces with increasing A, indicating the onset of homogeneous explosion phenomena. The effect of geometry diminishes at sufficiently low heating rates, which removes the effect of the conduction terms such that, in the limit, the E' curves will end at their respective explosion points and intersect the unity ratio line.

With respect to constant  $\epsilon_c$  curves, one can observe the change in vertical position as well as a higher dependence on external heat flux for the present two-dimensional case compared to the one-dimensional case. Both accentuate parame-

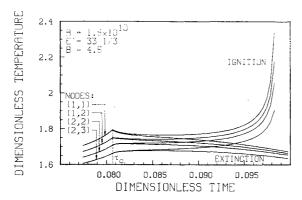


Fig. 8 Sensitivity of corner temperatures to duration of heating for low activation energy  $E^\prime$ .

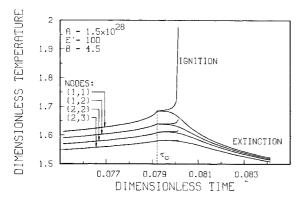


Fig. 9 Sensitivity of corner temperatures to duration of heating for large activation energy E'.

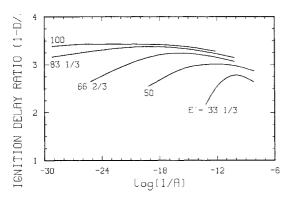


Fig. 10 Ratio of ignition times of one-dimensional to two-dimensional geometry vs log(1/A) for constant activation energy E'.

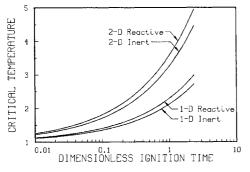


Fig. 11 Critical dimensionless temperature  $\theta_c$  vs dimensionless ignition time  $\tau_c$  for one-dimensional and two-dimensional geometries; inert and reactive cases.

ters responding to the geometry effect, which produces higher rates of heating and hence more rapid reactant consumption in the corner region. The closer spacing of  $\epsilon_c$  curves and the more dominant effect of fraction reacted on the attainment of ignition for the two-dimensional case are explained by the two-dimensional geometry. Thus this geometry effectively causes very localized ignition behavior.

Comparison of the plots displaying the dependence of  $\theta_e$  on A and E' shows that all curves are shifted upward uniformly to a small extent for the present case. This small temperature increase can be anticipated as being necessary because of the higher cooling rates after flux cessation in the corner geometry.

Figure 11 shows  $\theta_c$  vs  $\tau_c$  for both geometries using interrupted heating data. Shown are Eqs. (4) and (5) as well as one-dimensional results generated from Eqs. (10) and (11) from Bradley's<sup>4</sup> paper. The vertical spacing of corresponding reactive curves clearly illustrates the effect of geometry.

Comparison of Fig. 12 to Fig. 6 of Ref. 4 reveals substantially higher critical temperatures at high values of parameter AE', expressed as  $Rq^2/QvkE$  in dimensional quantities. This difference can be attributed to differences in temperature distributions as a function of initial temperature for the two geometries. The differences in heat transfer characteristics are most prominent at low initial temperatures and high rates of heating.

A correlation equation relating the ignition delay  $\tau_e$  to system parameters A and E' was determined to be very similar to those found in Refs. 3 and 4 as

$$A = C(E')^{1/2} \cdot \left[ 1 + 4(\tau_c/\pi)^{1/2} \right]^{-1} \times (\pi \tau_c)^{-1/4} \cdot \exp\left\{ E' / \left[ 1 + 4(\tau_c/\pi)^{1/2} \right] \right\}$$
 (7)

where C was found to be  $5\pm15\%$ , correlating data in Figs. 3 and 4 within 4%. The factor 4 multiplying the  $\tau^{1/2}$  term arises from the inert heating solution for the current two-dimensional case, and the factor C is increased from the one-dimensional result of 0.65. Otherwise, the form of the predictive equation is identical to the one-dimensional case, interestingly enough.

The present results may be compared to experimental work by Baer and Ryan,<sup>2</sup> who proposed a simple ignition theory where thermal runaway was governed by a single exothermic surface reaction. Their experimental check for one-dimensional and two-dimensional geometries indicated a reduction in ignition times from 3.0 to 3.6 for an E' of 462/3 and a heat flux ranging from 83.6 to 543.4 kW/m² (2 to 13 cal/cm²-s). Their numerically predicted reduction in ignition delay of 3.6, larger than the present results, is caused by the chemical reactivity being limited to the surface, whereas presently a bulk heat generation rate is assumed.

## Discussion

The results of the present investigation are limited in two respects, mathematically and physically. Inaccuracies in the numerical procedure are not considered serious based on detailed computations to justify the use of the inert closed-form solution during the initial heating phase.<sup>6</sup> The spatial grid size was selected such that calculations at a doubled spatial increment resulted in a maximum increase of 3% in critical heating times. The imposition of insulated boundary conditions to approximate the infinity conditions resulted only in a small accumulation of energy in this insulated corner region. Its effect back at the exposed corner is confirmed to be negligible because of the existence of very high gradients in this region.

The infinitely sharp corner represents a physically impossible configuration, since a small yet finite radius of curvature is surely present in real propellants. The inclusion of a radius of curvature of the order of a few micrometers, being a typical dimension of a small AP crystal, may produce a more

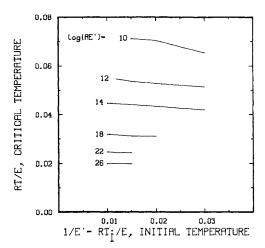


Fig. 12 Effect of initial temperature on critical temperature tor parameter  $AE' = Rq^2/QvkE$ .

realistic model. Current results may be interpreted as ignition initiating locally at microscopic surface irregularities.

Further physical limitations include the constant thermal properties assumption, the representation of the complex chemistry by a single Arrhenius reaction rate, and the solid phase mechanism controlling the ignition process.

Although the nondominant role of a purely solid phase reaction governing the ignition process is well established in the literature for both types of propellants, it is reported that under certain conditions ignition predictions computed via a solid phase theory may agree closely with experiments.  $^{9,10}$  These conditions refer to physical circumstances such as low heat flux levels, high ambient oxidizer concentration, and high pressure.  $^{10}$  Time scales associated with the inert heating time are frequently much larger here than those occurring in the gas phase, such as the diffusion and chemical reaction time scales. Experimental plots showing ignition delay vs heat flux level with slopes less negative than -2 are in full qualitative agreement with solid phase theory results.  $^9$  The good agreement reported between the experiment and numerical predictions lends further credibility to the ignition process controlled by solid phase mechanisms.  $^2$ 

With full knowledge of the limitations and idealizations of the model used, it was felt that an initial major numerical investigation in the effects of geometry on the ignition characteristics of solid propellants was best served by employing a simple solid phase mechanism as the ignition controlling agent. As such, the current results present a fairly complete picture of critical conditions and comparison to Bradley's<sup>4</sup> work permitted the evaluation of geometrical and chemical effects within the framework of these overly simplified models.

#### **Conclusions**

Ignition times are significantly reduced when sharp corners are present on a surface to be ignited, reductions ranging by factors of 2.5 to 3.4 for identical parameter values. Slightly higher temperatures occur for the corner geometry at identical parameter settings for A, B, and E' which are necessary to overcome higher cooling rates existing in the two-dimensional case as a result of shorter heating times and therefore steeper thermal gradients. The ignition process is more sensitive to heat release parameter B for the present case as is indicated by the closer spacing of critical iso-consumption curves and the reduced time range where ignition is still possible.

## Acknowledgment

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