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TRANSIENT COMBUSTION: MODELS VS ONERA DATA

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20. Abstract (Cont'd):

Predictions of very steep runaway transients were shown to be either a linearly unstable initial condition, or unreproducible by any method.

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I. INTRODUCTION

Solid propellant burning rate is usually assumed to depend only on pressure for the convenience of the design engineer. There remains, however, the nagging suspicion that things are probably not that simple. Although fast digital computers have obviated the need for simple algebraic expressions ($r=ap^n$), we have given only a little attention to the possibility that the burning rate dependence may extend to other variables such as rate of pressurization, pressure history, or stress history in the solid. In high performance applications, burning rate may then be fully transient (read: quasi-steady treatment is inadequate).

Even if transient combustion exists, however, its effect on internal ballistics is still in doubt. Catastrophies of overpressure have had at least one other credible explanation: igniter operation, slow ignition, bed permeability, grain fracture. Any prediction of transient burning has had a serious limitation: quasi-steady flame in rapid pressure change, arbitrarily simple (or ignored) chemistry. Experimental evidence of transient burning is practically nonexistent. And without demonstrable evidence of a measurable effect, the theories will not compete with the ignition and mechanical explanations.

Predictions of transient combustion have come from models. One experiment with clear results was conducted by the French ONERA (Office National d'Etudes et de Recherches Aérospatiales).¹ The pressure changes were easily measured, the data reduction was uncomplicated, propellant properties were reported, and the results were reproduced in tests with more than one propellant. It is an experiment against which models can be measured.

Models are many. Unfortunately, the few that address the monotonic sharply rising pressure do not agree. The most popular approach is the thermal theory where the thermal condition of the solid dominates the burning rate response which depends on surface temperature.

Krier² pioneered the thermal theory approach. Kooker and Nelson³ used it to calculate sharp transient responses in a gun pressurization and Kooker⁴ used it for unsteady rocket motor calculations. All assumed uniform spatial heat release to integrate the flame energy equation to determine the heat

¹J. Brulard, P. Kuentzmann, and R. Kling, "Reponse d'un Propergol Solide a un Echelon de Pression," *La Recherche Aerospatiale*, Vol. 5, pp. 279-287, 1975.

²H. Krier, J. T'ien, W. Sirignano, and M. Summerfield, "Nonsteady Burning Phenomena of Solid Propellants: Theory and Experiments," *AIAAJ*, Vol. 6, pp. 278-285, 1968.

³D. Kooker and C. Nelson, "Numerical Solution of Solid Propellant Transient Combustion," *ASME J Heat Transfer*, Vol. 101, pp. 359-364, 1979.

⁴D. Kooker and B. Zinn, "Triggering Axial Instabilities in Solid Rockets: Numerical Predictions," *AIAA Paper 73-1298*, 1973.

feedback at the propellant surface. Summerfield, et al,⁵ used the Zeldovich heat feedback approach which avoided any specification of the flame structure. Nelson⁶ showed that for the same gun pressurization rate, the Krier approach and the Zeldovich approach predicted quite different transients.

Kumar and Kuo⁷ used the Zeldovich approach to predict a runaway regression rate for constant pressurization rate. In contrast, Nelson⁶ and Caveny⁸ found only modest excursions.

This report will apply such models to the ONERA transient burning experiment.

II. THE MODELS

Thermal theory models all solve the transient heat conduction problem in a semi-infinite, inert solid

$$\rho c \left[\frac{\partial T}{\partial t} + r \frac{\partial T}{\partial x} \right] - \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) = 0 \quad , \quad -\infty < x < 0 \quad . \quad (1)$$

In the convective term, the regression rate (r) depends on the surface temperature (T_s) which makes the equation nonlinear and analytically intractable.

Usually the thermal properties are assumed constant and the equation reduces to

$$\frac{\partial T}{\partial t} + r \frac{\partial T}{\partial x} - \alpha \frac{\partial^2 T}{\partial x^2} = 0 \quad . \quad (2)$$

Allowing temperature dependence of the properties produces no startling deviations.⁹

⁵M. Summerfield, L. Caveny, R. Battista, N. Kubota, Y. Gostinsev, and H. Isoda, "Theory of Dynamic Extinguishment of Solid Propellants with Special Reference to Nonsteady Heat Feedback Law," J Spacecraft and Rockets, Vol. 8, pp. 251-258, 1971.

⁶C. Nelson, "Response of Three Types of Transient Combustion Models to Gun Pressurization," Combustion and Flame, Vol. 32, pp. 317-319, 1978.

⁷M. Kumar and K. Kuo, "Dynamic Burning Effects in the Combustion of Solid Propellants with Cracks and the Use of Granular Bed Combustion Models," Naval Weapons Center Report TP-6193, 1980.

⁸L. Caveny, M. Summerfield, and C. Nelson, "Ignition Transients and Pressurization in Closed Chambers," BRL Memorandum Report 2558, 1975 (AD A017747).

⁹C. Nelson, "Transient Combustion Calculations with Variable Thermal Properties," BRL Report ARBRL-TR-02294, 1981 (AD A098657).

The regression rate is assumed to depend only on surface temperature in an exponential with two constants

$$r = A_s \exp (- E_s / R_u T_s) . \quad (3)$$

This commonly assumed form fits either a sublimation or a pyrolytic gasification but details of the gasification are too poorly known to assign firm values to the two constants, pre-exponential (A_s) and activation energy (E_s). Surface temperature varies continuously and comes from the solution of the conduction equation.

The initial condition is a given regression rate (r_0) and a given temperature distribution in the solid. A frequent condition is steady state burning with constant propellant properties for which the initial condition is the well known

$$T = T_0 + (T_s - T_0) \exp (rx/\alpha) . \quad (4)$$

Other conditions occur occasionally such as variable properties⁹ or cold solid.⁸

The boundary condition far into the semi-infinite solid is the constant initial temperature,

$$T(-\infty, t) = T_0 . \quad (5)$$

The surface boundary condition distinguishes the models. Heat feedback from the flame and from any exothermic reaction at the solid surface combine to form a gradient boundary condition

$$\frac{\partial T}{\partial x} \Big|_s = g (r, T_s, p, \dots) . \quad (6)$$

The Krier type condition of uniform heat release in the flame is typified by the Kooker model⁴ where

$$\frac{\partial T}{\partial x} \Big|_s = Z_1 Q_s r + Z_2 Q_f p^m / r . \quad (7)$$

Z_1 and Z_2 are constants which depend on the thermal and physical properties.

The Zeldovich approach⁸ leads to

$$\frac{\partial T}{\partial x} \Big|_s = \frac{r}{\alpha} [T_s - T_0 - \frac{1}{\sigma_p} \ln (r/r_s)] . \quad (8)$$

A flame sheet assumption where all the heat release occurs at the final flame temperature is common in nitrocellulose base propellants studies. The boundary condition there is

$$\frac{\partial T}{\partial x} \Big|_s = Z_3 r (T_s - T_f) + Z_4 Q_f p^m / r . \quad (9)$$

Z_3 and Z_4 are also constants depending on physical properties.

Note that both Eq. (7) and Eq. (9) assume that the heat release term in the gas phase depends on the instantaneous pressure

$$w = w_o p^m \quad . \quad (10)$$

The cause for change is a changing pressure which is imposed on the combustion. In some applications the pressure may come from a coupled solution of the chamber conditions. In the present application it is simply imposed as the ONERA measured pressure history.

III. NUMERICAL METHODS

It is first convenient to transform the problem into nondimensional variables. Kooker's transformation³ is convenient.

$$\tau = t (r_o^2/\alpha) \quad . \quad (11)$$

$$\eta = x (r_o/\alpha) \quad . \quad (12)$$

$$\theta = (T - T_o) / (T_{so} - T_o) \quad . \quad (13)$$

$$H = Q_s / [c_s (T_{so} - T_o)] \quad . \quad (14)$$

$$E = E_s / (R_u T_{so}) \quad . \quad (15)$$

$$A = E (1 - T_o/T_{so}) \quad . \quad (16)$$

$$P = p/p_o \quad . \quad (17)$$

The new equations are

$$\frac{\partial \theta}{\partial \tau} + R \frac{\partial \theta}{\partial \eta} - \frac{\partial^2 \theta}{\partial \eta^2} = 0 \quad , \text{ and} \quad (18)$$

$$R = \exp [A(\theta_s - 1) / (1 + A/E (\theta_s - 1))] \quad . \quad (19)$$

The initial condition is

$$\theta(\eta, 0) = \exp(R\eta) \quad . \quad (20)$$

The cold boundary condition is

$$\theta(-\infty, \tau) = 0 \quad . \quad (21)$$

The surface boundary condition for each model is as follows:

1. Kooker

$$\frac{\partial \theta}{\partial \eta} = R[H + (\theta_s - 1)(1 - c_p/c_s)] + (1-H) P/R^m \quad . \quad (22)$$

2. Zeldovich

$$\frac{\partial \theta}{\partial \eta} = R \left[\theta_s - \left(\frac{1}{\sigma_p (T_{so} - T_o)} \right) \ln (R/R_s) \right] \quad (23)$$

3. Flame Sheet

$$\frac{\partial \theta}{\partial \eta} = R \left[H + (\theta_s - 1) - (c_p/c_s)(\theta_f - 1) \right] + Z_5 P^m / R \quad (24)$$

Z_5 is another constant depending on physical properties.

The numerical solution used an implicit method with a tridiagonal matrix inversion. Kooker and Nelson⁶ showed this method was competitive with other implicit methods although it suffers a small error when the grid spacing varies greatly from one end of the grid to another, but the resultant accuracy loss is small.

Numerical accuracy was aided by using a three-point backward difference scheme at the surface. Accuracy and efficiency were combined by using a grid spacing which varied inversely with the expected temperature gradient, small at the surface and growing with distance into the interior. The surface grid spacing was varied over the range $.0005 < \Delta \eta < .023$ with no useful effect on accuracy. Errors of 10^{-7} to 10^{-10} in the residual of Equation (18) were small compared to the smallest term in the conduction equation which was of order one. With typical values the smallest grid spacing allowed cell-to-cell temperature differences of only about 0.1 K at the surface. The combination of time step and grid spacing produced values of the stability parameter $(\Delta \tau / (\Delta \eta^2))$ ranging from 0.05 to 200 with little effect. (An explicit scheme must not exceed 0.5.)

Equation (18) was linearized by guessing the regression rate and iterating until successive solutions converged in both surface temperature (θ_s) and regression rate (R). Convergence criteria were 10^{-8} for the surface temperature and 10^{-7} for the regression rate (both of order one). Relaxing that convergence criterion to as large as 10^{-4} had no appreciable effect on the solution when results were compared with ONERA combustion.

IV. THE ONERA EXPERIMENT

The ONERA apparatus is shown in Figure 1. Two independent steady pressure combustion chambers are separated by a passage blocked by a shear disc. In Figure 1 the white areas are the combustion gases, and the speckled areas are the burning solid propellant. The propellant geometry is unimportant. When both chambers reach steady pressure, the shear disc is ruptured to produce two experiments - a pressurization and a depressurization. The depressurization chamber starts at about 70 bars, and the pressurization chamber at about 20 bars. (Figures 1 through 4 are reprinted from the ONERA paper.¹)

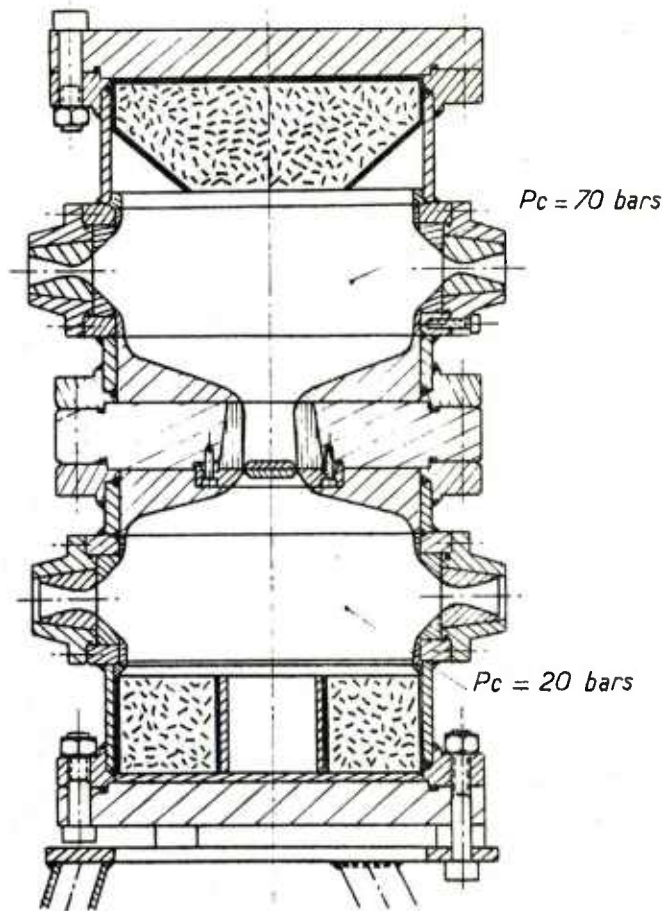


Figure 1. ONERA Apparatus

Pressure change rates were low by gun standards. The rate in the low pressure chamber was about 10^5 MPa/s compared to about 10^6 MPa/s in a tank gun.

A quasi-steady analysis reduced the pressure time history to instantaneous regression rate. Typical plots of regression rate-time is shown in Figures 2 and 3 for a positive pressurization. The line $\bar{v}_b$ shows the quasi-steady pressure dependent regression rate.

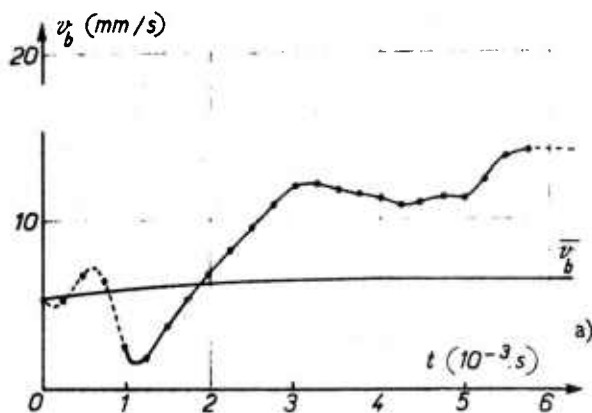


Figure 2. Regression Rate, Test 7

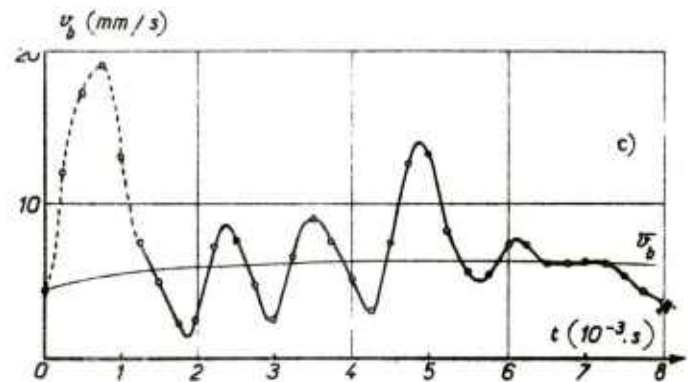


Figure 3. Regression Rate, Test 9

Data after about 3 ms should be ignored because the assumed choked flow through the passage no longer applies.

The figure of merit in the experiment is relative regression rate [instantaneous rate divided by quasi-steady rate ($\bar{v}_b$)]. Figure 4 shows the time dependence of the relative rate in the pressurization chamber for three distinct tests. It is this result that the models seek to duplicate. Note that the dotted curve on Figure 4 is not an experimental result; it should be ignored in the context of this paper. Note further that there is some discrepancy between the plots in Figures 2 and 3 and in Figure 4. Figure 3 particularly is not typified by the curves of Figure 4. Nevertheless, Figure 4 is the reported result.

The propellants were composites. Their physical and chemical properties as reported by Brulard¹ are:

Density, kg/m^3 , ρ	1735
Heat Capacity, J/kg K , c_s	1318
Initial Temperature, K , T_0	293
Conductivity, J/mKs , λ	0.46*
Temperature sensitivity, $\%/K$, σ	0.15
Surface activation energy, kcal/mol , E_s	25.83
Reference surface temperature, K , T_{so}	1000
Regression rate pressure exponent, n	0.15

The physical and thermal properties can easily be accepted. The combustion properties are open to more debate. Temperature sensitivity and pressure exponent can be directly measured and thus accepted. Activation energy and surface temperature are subject to doubt. Direct measurement of the activation energy would require measurement of a 12K surface temperature change as pressure increased from 25 to 80 bars. (Regression rate increases from 6 to 7 mm/s.) Whether the reference surface temperature is accurate is of only minor importance for the models; the changes from it dominate regression rate transients at such a high activation energy.

Some models also need the surface heat release to obtain the non-dimensional variable (H). For double base propellants Kubota¹⁰ inferred values of 0.7 to 0.8 for H varying inversely with regression rate. Kooker⁴ used values in the same range based on inference from Beckstead, et al,¹¹

* Private communication, J. Brulard, 1976.

¹⁰N. Kubota, T. Ohlmiller, L. Caveny, and M. Summerfield, "Site and Mode of Action of Platonization in Double Base Propellants," *AIAAJ*, Vol. 12, pp. 1709-1714, 1974.

¹¹M. Beckstead, R. Derr, and C. Price, "A Model of Composite Solid Propellant Combustion Based on Multiple Flames," *AIAAJ*, Vol. 8, pp. 2200-2207, 1970.

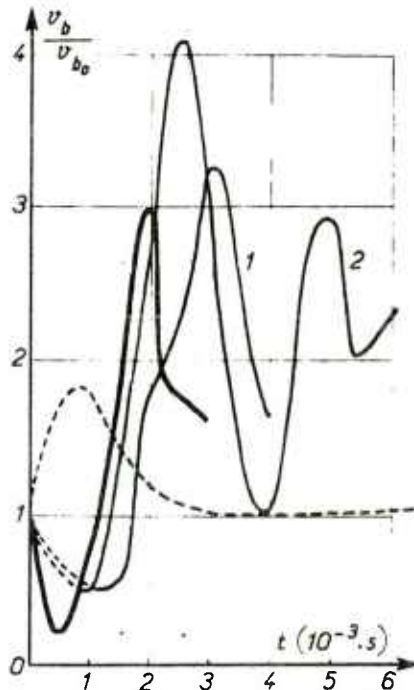


Fig. 13. — Comparaison de diverses réponses à l'échelon positif.
 — Combustion radiale (composition sans aluminium).
 — Combustion frontale 1 et 2.
 - - - - - Référence [11].

Figure 4. Relative Regression Rates, ONERA

V. RESULTS

The models do not reproduce the ONERA regression rates. No calculated excursion even doubled the quasi-steady regression rate which the experiment found to be 3-4 times the quasi-steady rate.

Kooker Model

The Kooker model predicted only a 50% excursion for the nominal propellant properties. Higher activation energies or higher surface heat release typically enlivens responses.¹² Pushing both higher did, indeed, produce a sharp excursion but of questionable credibility. The peak regression rate was either less than 2 or more than 30. The jump occurred in a narrow range with no apparent middle ground. Figures 5 and 6 show the jump. Note the ordinate is nondimensional rate (instant rate/quasi-steady rate).

¹²D. Kooker and C. Nelson, "Numerical Solution of Three Solid Propellant Combustion Models During a Gun Pressure Transient," BRL Report 1953, 1977 (AD A035250).

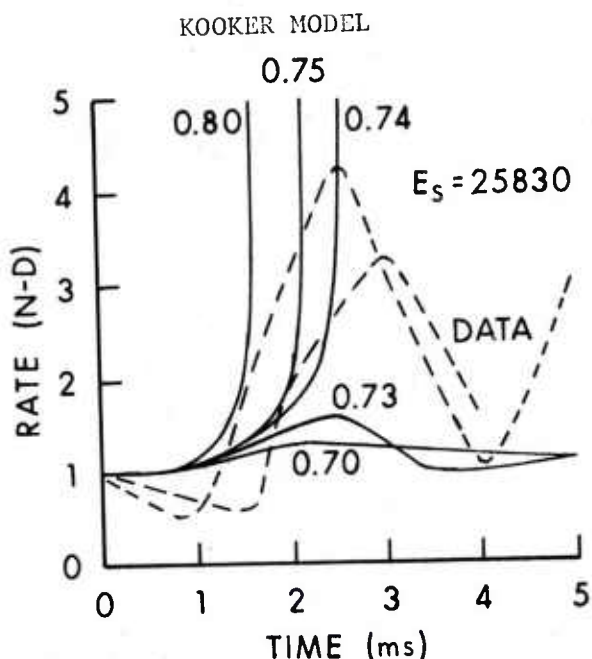


Figure 5. Effect of Surface Heat Release, Kooker Model

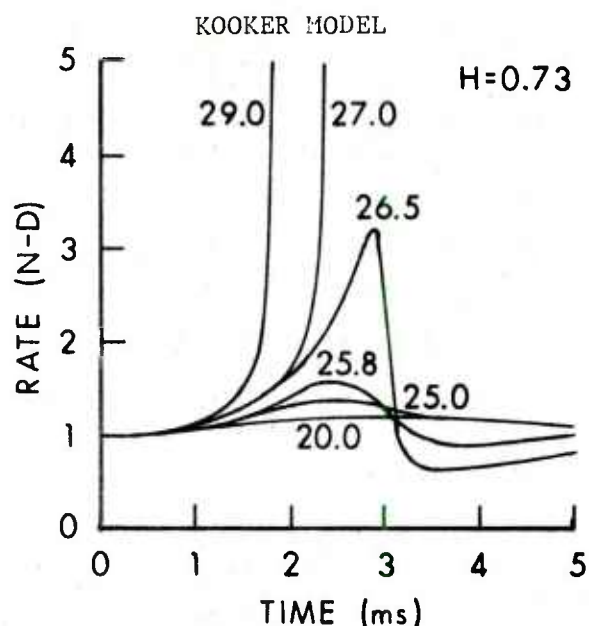


Figure 6. Effect of Activation Energy, Kooker Model

Figure 7 shows the combination of E_s and H which forms the boundary between high and low excursion. The sharp transition, if physical, would bode ill because reasonable experiments cannot distinguish such fine differences in either variable.

This behavior contrasts with earlier findings¹² that the peak relative rate varies continuously with heat release although those findings were at a lower activation energy (15 kcal/mol) and faster pressure rise (10^6 MPa/s).

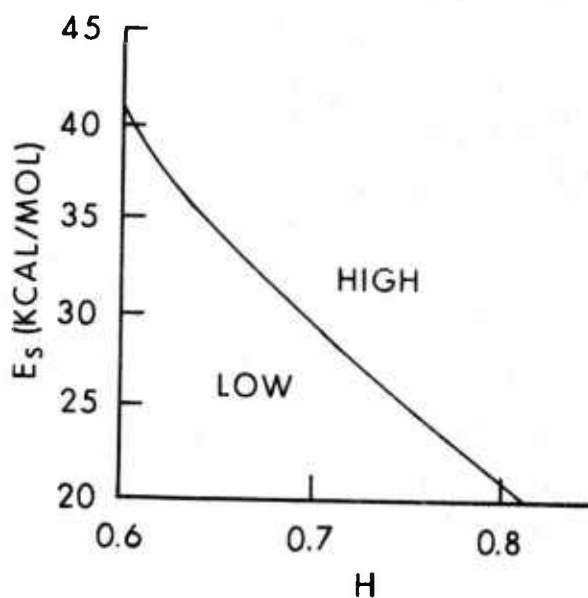


Figure 7. Transition Boundary, Kooker Model

An explanation arises from linear stability consideration. Kooker³ showed that some initial conditions are inherently unstable. With no disturbance to the initial condition (like pressure change), a spiking response can be generated merely by a disturbance as small as errors in the computation.* And, indeed, exactly that happened; see Figure 8 where constant pressure produced spikes for nominal E_s (25830) and high H (0.8) - a point in the high response region of Figure 7.

Figure 8 says that calculations of transients in the high response region of Figure 7 cannot be trusted.

Zeldovich Model

The Zeldovich approach calculated no transient over about 20%. Increasing the activation energy (E_s) to as much as 50 kcal/mol could not induce a great excursion, either.

The parameter which most rapidly affects transients in the Zeldovich model is the temperature sensitivity. The heat feedback has an excursion correction term which is inversely proportional to the temperature sensitivity. If temperature sensitivity is treated parametrically to test the effect of its variation, Figure 9 results.

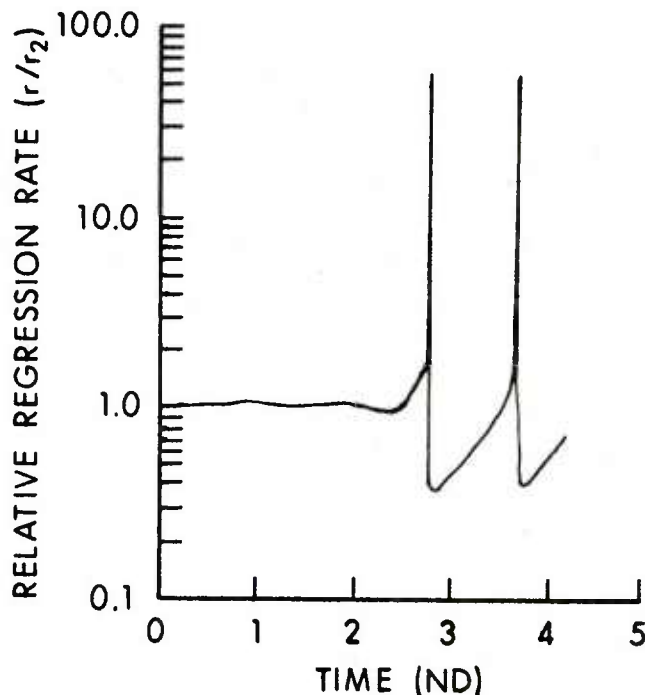


Figure 8. Unstable Case, Constant Pressure

*Thanks to D.E. Kooker for pointing out the possibility of the linear instability.

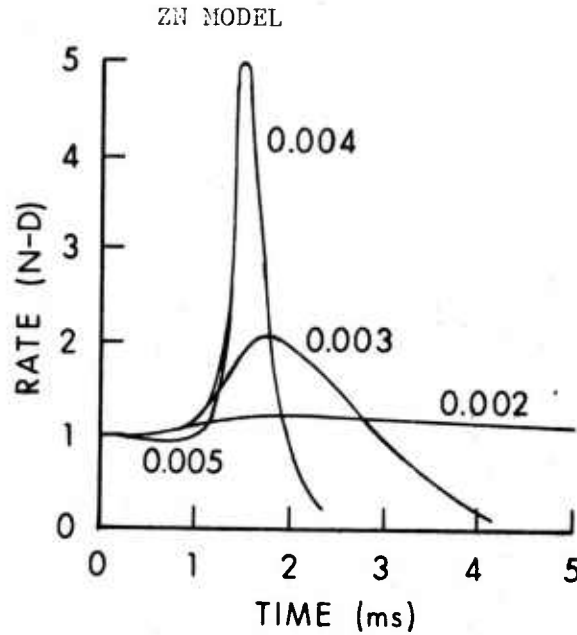


Figure 9. Effect of Temperature Sensitivity, Zeldovich

At high temperature sensitivity the excursions can be created; but they are followed by extinguishment, which the propellant did not see.

The same behavior occurs when the temperature sensitivity is raised, and activation energy is varied. Figure 10 shows that result.

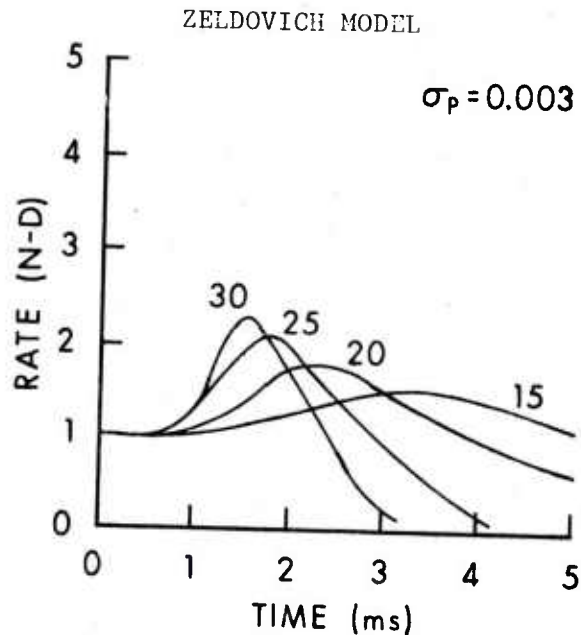


Figure 10. Effect of Activation Energy, Zeldovich

Flame Sheet Model

The flame sheet model calculated no excursions over 2%. Such a result could have been foreseen by noting that when the flame reaction rate varies with P^{2m} the two terms in the heat feedback boundary condition of Equation (9) cancel, and steady state is assured.

VI. DISCUSSION

The models failed to reproduce the experimental results. Which is wrong - model or experiment? Being unwilling to challenge the data, we will assume something is amiss with the models.

Quasi-Steady Flame

The concept of an inert solid allows the heat conduction to govern the solid interior temperature profile. Propellants with high enough activation energy to be stable before ignition would be inert except close to the surface if heat conduction is the only mechanism of energy transfer to the unreacted solid. The most likely candidate for error, then, is the surface heat release or the flame.

The quasi-steady flame is only a convenience. It depends on an argument that the characteristic time for pressure change (.001 sec in this experiment) is larger than the flame characteristic time (order 10^{-5} sec), as in Summerfield.⁵ In a gun problem where the pressure characteristic time is closer to 10^{-5} sec, the quasi-steady flame is less appealing although it is still fast with respect to the solid. But for the ONERA experiment it seems a justifiable assumption.

The form of the steady gas phase chemistry may be incorrect. Neither of the two extremes, uniform or flame sheet, gave the correct answer. Perhaps some intermediate approach, or some combination approach like Merkle, et al,¹³ could help. At least it adds more adjustable constants. Miller's idea¹⁴ of a quasi-constant heat release is an alternate version of a uniform release.

Using an unsteady gas phase would add complications. A description of the flame would require kinetics and transport information not generally available and a substantial increase in computing. Suhas and Bose¹⁵ attempted a less rigorous step by postulating that transients in blowing increased the

¹³C. Merkle, S. Turk, and M. Summerfield, "Extinguishment of Solid Propellants by Depressurization: Effects of Propellant Parameters," AIAA Paper 69-176, 1969.

¹⁴M. Miller, "An Idealized Model of Homogeneous Solid Propellant Combustion," Combustion and Flame, Vol. 46, pp. 51-73, 1982.

¹⁵H. Suhas and T. Bose, "A Mathematical Model to Predict Transient Burning Rate and Decay Rates for Extinction of Composite Propellants," Combustion and Flame, Vol. 28, pp. 145-153, 1977.

heat transfer to the surface in direct proportion to the blowing; i.e., a pressure decrease caused a regression rate increase. One consequence of that approach was that the positive pressurization reduced the regression rate which never recovered to the initial rate. No positive excursion would result from that theory.

Zeldovich

The Zeldovich model predicts only small excursions for this low temperature sensitivity propellant. Earlier calculations^{6,8} also produced only low excursions. If the temperature sensitivity could be a variable, it would be easier to adjust calculation to experiment. But it is an independently physically measured variable and not subject to arbitrary assignment.

The tendency to excursions at high temperature sensitivity with Zeldovich can be seen in Zeldovich stability diagram as shown by Stokes.¹⁶ For constant E_s , Figure 11 shows the transition from stable to unstable burning as temperature sensitivity increases from 0.1% to 0.4%. And this trend to instability is confirmed in calculations of extinguishment when the temperature sensitivity was in the unstable region of the diagram.

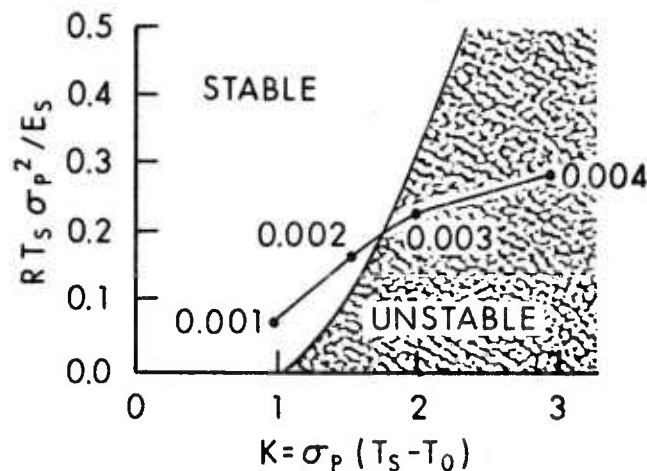


Figure 11. Zeldovich Stability Diagram

Only one investigator has found large transients with the Zeldovich approach. Kuo⁷ calculated runaway regression rates for pressurization at 10^5 - 10^6 atm/s of composite propellant. Unfortunately, his results could not be reproduced with the method described here despite the fact that the

¹⁶B. Stokes, "Application of Zeldovich Heat Feedback to Dynamic Burning of Throttleable Fuel-Rich Propellant Fuel Generators," *Astronautica Acta*, Vol. 18, pp. 395-407, 1973.

equations and the implicit solution are the same. The time and space discretization are somewhat different, but variation over a wide range of Δn and Δt produced no hint of any substantially higher transient. The present method can calculate spikes even as steep as in Figure 8. Krier's calculated runaway² was later shown to be bounded,³ but it did have a spike which the numerical method could calculate. The inference is that the method would find a spike if it were a solution to the differential equation (a separate question from whether it is physically correct).

An entirely different integration scheme, invariant imbedding, also failed to reproduce Kuo's results. A second suspicious aspect of Kuo's result is that the runaway occurs at about the same pressure regardless of the pressurization rate (2.4 times the initial pressure). Unless Kuo's results can be verified, it seems that the Zeldovich approach will not calculate high transients for low temperature sensitivity propellants.

Initial Lag

The models do not capture the initial drop in relative regression rate shown in the ONERA results of Figure 4. Such a result is consistent with the low positive excursions later because other calculations with these models showed an initial relative regression rate lag as a prelude to a positive excursion. Generally, the higher the positive excursion, the lower the initial negative excursion. Nelson⁹ found a lag up to 50% at very high pressurization rate (7×10^5 MPa/s) with the Zeldovich model but only a 10% lag at 7×10^3 MPa/s. Kooker found only a small initial lag at 7×10^3 MPa/s. The low ONERA pressurization rate of 10^3 MPa/s should produce only a small lag. An initial lag is not surprising; the ideal thermal theory model assumes a lag. It is possible that the ONERA data reduction exaggerated the initial response by overlooking some transient aspect of the first compression wave to enter the low pressure chamber.

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LIST OF SYMBOLS

a	regression rate coefficient
A	constant in regression rate (n-d)
A_s	pre-exponential in regression rate
c_s	heat capacity of solid
c_p	heat capacity of gas
E	surface activation energy (n-d)
E_s	surface activation energy (n-d)
H	surface heat release (n-d)
m	pressure exponent in flame reaction
n	regression rate exponent
p	pressure
P	pressure (n-d)
Q_f	flame heat release
Q_s	surface heat release
r	regression rate
r_o	reference regression rate
r_s	quasi-steady regression rate
R_s	quasi-steady regression rate (n-d)
R	regression rate (n-d)
R_u	universal gas constant
T	temperature
T_s	surface temperature
T_o	cold solid temperature
T_{so}	reference surface temperature
w	flame reaction rate
w_o	reference flame reaction rate

x	distance coordinate
Z	constant
α	thermal diffusivity
η	distance coordinate (n-d)
σ_p	temperature sensitivity of regression rate
λ	thermal conductivity
τ	time (n-d)
θ	temperature (n-d)
θ_s	surface temperature (n-d)
θ_f	flame temperature (n-d)

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