Defence Science Journal, Vol 46, No 5, November 1996, pp 425-433

# Simulation of Combustion of Melting Energetic Materials

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## ABSTRACT

To simulate the combustion of energetic materials (EM) with melting and surface evaporation, a one-dimensional transient model is formulated. In condensed phase, the model considers heat propagation and EM decomposition via a first order reaction. In the gas phase, it considers heat propagation, species diffusion, exothermic decomposition of vapour via a first order reaction and exothermic conversion of gas components via a second order reaction. The boundary condition at the liquid-gas interface corresponds to equilibrium evaporation described by the Clausius-Clapeyron equation. The effects of melting and exothermicity of condensed phase reaction on the stability of combustion are studied. When simulating radiative ignition, it has been revealed that it can occur in one, two or three stages with different regimes of heat feedback from the gas phase. With relatively slow deradiation, a gas flame approaches the burning surface and sustained combustion is governed by heat feedback from the gas flame with burning rate several times higher than the gasification rate. With fast deradiation at high radiant fluxes the combustion extinguishes, indicating the impossibility of stable ignition under high heating rates. The limitations and possible improvements to the model are considered.

## NOMENCLATURE

| | |
|---|---|
| $t$ | Time (s) |
| $x$ | Spatial coordinate (cm) |
| $r_b$ | Burning rate (cm/s) |
| $V$ | Gas velocity (cm/s) |
| $T$ | Temperature (K) |
| $\rho$ | Density (g/cm$^3$) |
| $p$ | Pressure (MPa) |
| $y_i$ | Mass fraction of species $i$ |
| $C$ | Specific heat of condensed phase [cal/(g.K)] |
| $C_{pi}$ | Constant-pressure heat capacity of species $i$ [cal/(g.K)] |
| $\lambda$ | Thermal conductivity [cal/(s.cm.K)] |
| $Q$ | Heat release per unit mass (cal/g) |
| $M_i$ | Molecular weight of species $i$ (g/mol) |
| $R$ | Universal gas constant [cal/(mol.K)] |
| $L$ | Latent heat of evaporation (cal/g) |
| $A$ | Pre-exponential factor $A_1$ ~ (l/s), $A_2$ ~ [cm$^3$/(mol.s)] |
| $E$ | Energy of activation (cal/mol) |
| $D$ | Diffusion coefficient (cm$^2$/s) |
| $q$ | External heat flux [cal/(cm$^2$.s)] |
| $f$ | Frequency of oscillations (l/s) |
| $\alpha$ | Extinction coefficient in Beer's law (l/cm) |

Received 02 September 1996

*Subscripts*

| | |
|---|---|
| $c$ | Parameters of the condensed phase |
| 1, 2, 3, | Species in a gas phase |
| $s$ | Propellant surface |
| $m$ | Melting point |
| $0$ | Initial condition |
| $st$ | Steady-state regime. Variables without index correspond to the bulk of gas. |

## 1. INTRODUCTION

The modern solid propellant formulations are based on novel energetic materials like ammonium dinitramide, hydrazine nitroformate, nitramines and energetic binders which melt and evaporate at the surface. The understanding of combustion mechanism of such materials provides a tool to develop up-to-date combustion models for composite solid propellants.

A steady-state combustion model of evaporating energetic materials (EM) was first proposed by Belyaev[1,2] for secondary explosives. In this model, the reactions occurring in the condensed phase have been neglected and surface temperature was assumed to be equal to the boiling temperature of the EM. For ammonium perchlorate, a stationary combustion model[3] has been developed taking into consideration partial depletion and equilibrium sublimation of condensed phase and assuming a negligibly small role of the gas phase reactions. The method of small perturbations has been employed[4,5] to study the stability of steady-state combustion regimes of EM with evaporation on the surface without reactions in the condensed phase and assuming the infinitely thin reaction zone in the gas phase. The up-to-date combustion models[6-9] take into account the global reactions in the liquid phase, the detailed reaction kinetics in gas, and non- equilibrium evaporation at the surface.

The last mentioned models show impressive agreement with experimental data on burning rate dependence on pressure and initial temperature. However, the calculations by these models are extremely complicated and time consuming. Therefore, they are mainly addressed to steady-state combustion regimes and do not allow to perform study of transient combustion in a broad range of parameters.

There is a need for a model with reasonably detailed description of chemistry and physics of combustion which could be used for qualitative investigation of transient combustion regimes of different types of energetic materials with melting and evaporation at the surface. In subsequent sections, we discuss the problem formulation and the results of calculations within the framework of such a model recently developed by our group. It is believed that step-by-step improvement of the model can be achieved by comparison with experiment.

## 2. PROBLEM FORMULATION

In this model, we deal with homogeneous semi-infinite solid material which melts at certain temperature and evaporates at the surface. The model considers heat propagation in solid and liquid phases with liquid material decomposition via a first order reaction . Specific heat and density are taken to be equal for solid and liquid materials but thermal conductivity coefficients are assumed different. The radiation absorption in the bulk of condensed phase is in accordance with Beer's law.

In the gas phase, the model considers heat propagation, species diffusion and exothermic decomposition of vapor via a first order reaction with subsequent conversion of intermediate products via a second order reaction that produces final combustion products.

On the interface between liquid and gas phases, phase equilibrium is assumed to be according to the Clausius-Clapeyron equation. Actually, there is no exact equality between the mass flow rates of evaporation $M_+^*$ and condensation $M_-^*$

$$M_+^* - M_-^* = y_{cs} m \qquad (1)$$

where $m$ is the mass burning rate; $y_{cs}$ is the mass fraction of vapour in total mass flow rate generated by the condensed phase. Equation (1) is known to be used for calculating $m$[6-9]. However, we consider the arguments[10] given in favour of equilibrium evaporation sufficiently convincing. Let us analyze the relationship obtained for the rates by division of Eqn(l) by gas density near the surface, i.e.

$$y_{1s}\left(V_+^* - V_-^*\right) = V y_{cs} \qquad (2)$$

Here $V$, $V_+^*, V_-^*$ are the gas velocity (the arithmetical mean velocity of all molecules both approaching and receding from the surface) and the mean velocities of molecules moving from the surface and falling on it, respectively; $y_{1s}$ is the mass fraction of vapour above the surface. The estimate can be made as

$$V/V_-^* << 1 \tag{3}$$

Indeed, $V_-^*$ is of the order of sound velocity. At surface temperature it amounts to hundreds of metres/second. Velocity of gas in EM combustion at atmospheric pressure is usually of the order of some metres/second which gives inequality (3). As pressure increases, $V$ increases. Equations (l) and (2) yield

$$M_+^*/M_-^* - 1 = V_+^*/V_-^* \;\; 1 = (V/V_-^*)(y_{cs}/y_{1s}) \tag{4}$$

In EM combustion, the condition $y_{1s} < y_{cs}$ holds due to the dilution of vapour near the surface by the combustion products from gas flame. However, for typical set of input parameters, the values $y_{1s}$, $y_{cs}$ are always of the same order of magnitude (the difference in case of the pronounced leading role of the gas phase amounts to 20-40%). Thus, from Eqns (3) and (4) it follows that

$$M_+^*/M_-^* - 1 << 1 \tag{5}$$

Using advanced approach one should take into account that a certain portion of falling molecules do not stick to the surface but is elastically reflected. This portion, however, is assumed to be small and taking it into account will not change a given qualitative estimate. Note that in[7] the sticking, coefficient is taken to be equal to unity.

Expression (5) confirms the validity of the Clausius- Clapeyron relationship for EM combustion conditions and shows the inconvenience of using Eqn(l) as a key expression for computing burning rate because it represents the difference of large numbers.

Hence, we assume that on the surface the following expression holds

$$(M/M_1)y_{1s}p \approx Ae^{-L/RT_s} \tag{6}$$

A mathematical model is formulated in the following way.

Let us choose movable coordinate system $(x, t)$ attached to the burning surface and formulate the system of equations describing combustion of EM with melting and evaporation:

(a) Solid phase $(x_m(t) \le x \le x_R)$

$$C_c \rho_c \left(\frac{\partial T_c}{\partial t} - r_b \frac{\partial T_c}{\partial x}\right) = \lambda_c \frac{\partial^2 T_c}{\partial x^2} + q_r(t)\, \alpha \exp(-\alpha x) \tag{7}$$

$$T_c(x, 0) = T_o,\; T_c(x_m, t) = T_m,\;\; at\;\; x = x_R,\; \partial T_c/\partial x = 0$$

b) liquid phase $(0 \le x \le x_m)$

$$C_c \rho_c \left(\frac{\partial T_c}{\partial t} - r_b \frac{\partial T_c}{\partial x}\right) = \lambda_c \frac{\partial^2 T_c}{\partial x^2} + \varphi_c + q_r(t)\, \alpha \exp(-\alpha x) \tag{8}$$

$$\rho_c \left(\frac{\partial y_c}{\partial t} - r_b \frac{\partial y_c}{\partial x}\right) = -\omega_c \tag{9}$$

$$\varphi_c = Q_c \omega_c;\;\; \omega_c = A_c \rho_c y_c \exp(-E_c/RT_c)$$

$$y_c(x_m, t) = 1,\; T_c(x, 0) = T_o,$$

$$T_c(x_m, t) = T_m,$$

$$-\lambda_c \frac{\partial T_c}{\partial x}\Big|_{x = x_m - 0} = -\lambda_c \frac{\partial T_c}{\partial x}\Big|_{x = x_m + 0} + Q_m\; V_m \rho_c$$

c) gas phase $(x_L \le x \le 0)$

$$C \rho \left[\frac{\partial T}{\partial t} + \left(V - r_b - \sum_{i=1}^{3} \frac{C_{pi}}{C} D_i \frac{\partial y_i}{\partial x}\right)\frac{\partial T}{\partial x}\right] = \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) + \varphi_1 + \varphi_2 \tag{10}$$

$$\rho\left(\frac{\partial y_1}{\partial t} + (V - r_b)\frac{\partial y_1}{\partial x}\right) = \frac{\partial}{\partial x}\left(\rho D_1 \frac{\partial y_1}{\partial x}\right) - \omega_1 \tag{11}$$

$$\rho\left(\frac{\partial y_2}{\partial t} + (V - r_b)\frac{\partial y_2}{\partial x}\right) = \frac{\partial}{\partial x}\left(\rho D_2 \frac{\partial y_2}{\partial x}\right) - \omega_2 + \omega_1 \tag{12}$$

$$\frac{\partial \rho}{\partial t} - r_b \frac{\partial \rho}{\partial x} + \frac{\partial(\rho V)}{\partial x} = 0 \tag{13}$$

$$p = R\rho TM \tag{14}$$

$$\frac{1}{M} = \left(\frac{y_1}{M_1} + \frac{y_2}{M_2} + \frac{y_3}{M_3}\right)$$

$$\varphi_1 = Q_1\omega_1;\;\; \varphi_2 = Q_2\omega_2;$$

$$\omega_1 = A_1 \rho y_1 \exp(-E_1/RT),$$

$$\omega_2 = \frac{A_2}{M_2}(\rho\, y_2)^2 \exp(-E_2/RT).$$

$$T(x,0) = T_0, \quad y_1(x,0) = y_2(x,0) = 0;$$

$$\text{at } x = x_L, \quad \partial T/\partial x = \partial y_1/\partial x = \partial y_2/\partial x = 0$$

Boundary conditions at x = 0 are as follows:

$$\lambda \frac{\partial T}{\partial x}\Big|_{x=-0} = \lambda_c \frac{\partial T_c}{\partial x} / \Big|_{x=+0} + {}^{q_r} - y_{cs}\,\rho_c\, r_b\, L$$

$$-\rho(V - r_b)\, y_{1s} + D_1 \rho \frac{\partial y_1}{\partial x} = \rho_c\, r_b\, y_{cs}$$

$$-\rho(V - r_b)\, y_{2s} + D_2 \rho \frac{\partial y_2}{\partial x} = \rho_c\, r_b\, (1 - y_{cs})$$

$$\rho(V - r_b) = -\rho_c\, r_b, \; y_{1s} = \frac{M_1}{M} \exp\left[-\frac{L M_1}{R}\left(\frac{1}{T_s} - \frac{1}{T_b}\right)\right]$$

Mass fraction of the combustion product and its effective diffusion coefficient are determined on the basis of mass conservation equation and condition of zero sum of individual diffusion fluxes:

$$y_1 + y_2 + y_3 = 1, \quad D_1 \frac{\partial y_1}{\partial x} + D_2 \frac{\partial y_2}{\partial x} + D_3 \frac{\partial y_3}{\partial x} = 0$$

In order to solve numerically the set of Eqns (7)-(14) with initial and boundary conditions, a spatial domain $x_L < x < x_R$ should be chosen on the basis of physical considerations or experiments. The data available in the literature on physical and chemical kinetics parameters of nitramines were taken as reference in the calculations.[10,11]

## 3. INSTABILITY OF STATIONARY COMBUSTION REGIMES

### 3.1 Effect of Melting

Nonlinear coupling between heat feedback from gas flame and thermal wave propagation in the condensed phase at certain values of parameters result in instability of stationary combustion of EM[12,13]. The analysis of small perturbations shows that in the presence of melting, the boundaries of combustion stability shift depending on three new parameters: relative value of melting latent heat, $q_m = Q_m/[c(T_{s,st}-T_o)$ relative value of melting temperature, $(\Theta)_m = (T_m-T_o)/(T_{s,st}-T_o)$, and ratio of EM thermal conductivities in solid and liquid states, $\Lambda = \lambda_c/\lambda_l$. A modified diagram of combustion stability is presented in Fig. 1. The curves drawn in coordinates $k_m = (\partial ln r/\partial T_o)(T_{s,st}-T_o + Q_m/c)$ and $r_N = \partial Ts/\partial To$ represent the boundaries of combustion stability. The domain above boundary corresponds to stable combustion regimes; that means that every small random perturbation of combustion wave parameters will decay in time. In particular, it is seen that the higher the relative melting temperature, broader the combustion stability domain. The effect of Λ-variation is relatively small. The effect of variation of $q_m$ had not been analyzed.

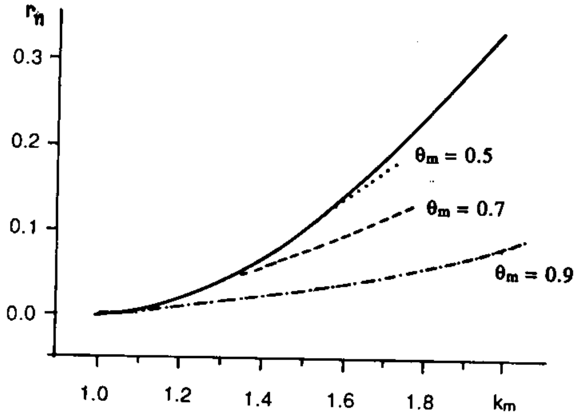

**Figure 1. Combustion stability map for melted EM. Solid line corresponds to EM without melting.**

### 3.2 Effect of Exothermicity of Condensed Phase Reaction

Numerical modeling revealed an intrinsic instability of steady-state regimes of combustion of EM with strong enough exothermic reaction in condensed phase and relatively weak heat feedback from the gas phase. In this case, the maximum temperature forms in the bulk of condensed phase that results in a local thermal explosion in subsurface layer. An example of temporal behaviour of burning rate in the course of ignition transients and appropriate spatial distributions of temperature and reacting components are shown in Fig. 2. The analytical study of combustion stability in the case of existence of temperature maximum in condensed EM revealed that steady-state combustion may occur only in restricted domain of determining parameters. The analysis has shown that at low evaporation latent heat, there is no overheat in the condensed phase. With high enough $Q_m$ and with the same heat feedback from the flame, the steady-state solution of energy equation with temperature maximum in subsurface layer becomes unstable to small perturbations. With further increase of $Q_m$, it is totally impossible to obtain steady-state solution because of

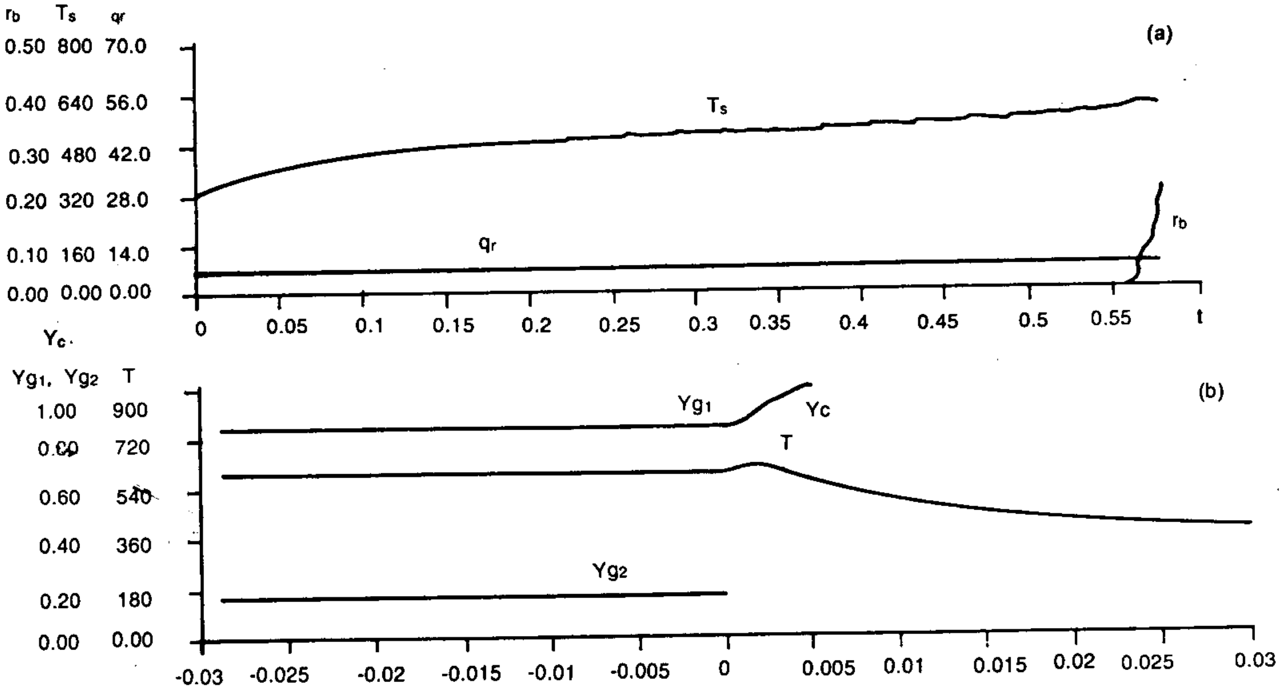

**Figure 2. Temporal (a) and spatial (b) ($t$ = 0.58 s) distributions of parameters in ignited EM. $A_1 \to 0$, $A_2 \to 0$.**

thermal explosion which develops in a subsurface layer. However, if for given propellant there is a coupling between burning rate and heat flux to the surface according to which a random increase of burning rate (velocity of gases issued from the surface) leads to decrease of heat feedback into condensed phase, there is a relatively small range of intermediate values of $Q_m$ when steady-state solution may exist .

## 4. RESULTS

### 4.1 Transient Combustion upon Radiative Ignition

The heating of EM by thermal radiation has been modelled as follows. For opaque EM ($\alpha = \infty$ in terms of Beer's law) we assumed the surface time-dependent heat release $q_r(t)$ which is constant $q_r = q_o$ within time interval $0 < t < t_1$ and linearly decreases to zero with $t_1 < t < t_2$. It appears that depending on the relation of parameters $q_o$, $t_1$, $t_2$ and chemical kinetics parameters (the gas phase, first of all) there are possibly one-, two- or even three-stage ignition regimes. All regimes have the same beginning, i.e. "inert" heating when all reactions may be neglected. This stage continues till the surface temperature reaches the EM boiling (a bit lower) temperature $T_b$. When $T_s$ approaches $T_b$, the rates of evaporation from surface and reactions in liquid and gas are noticeable.

One-stage ignition is realized with sufficiently strong heat release of reactions in the gas phase, in the time range $0 < t < t_1$ (Fig. 3). The gas flame is established in close vicinity of surface and provides heating and evaporation of the condensed phase. When $q_r$ gradually vanishes, the steady-state regime of

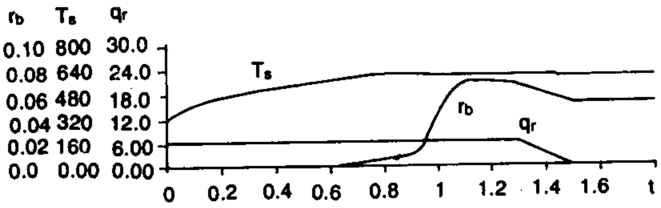

**Figure 3. One stage ignition ($q_o$ = 6.5 cal/cm$^2$s, $t_1$ = 1.3 s, $t_2$ = 1.5 s).**

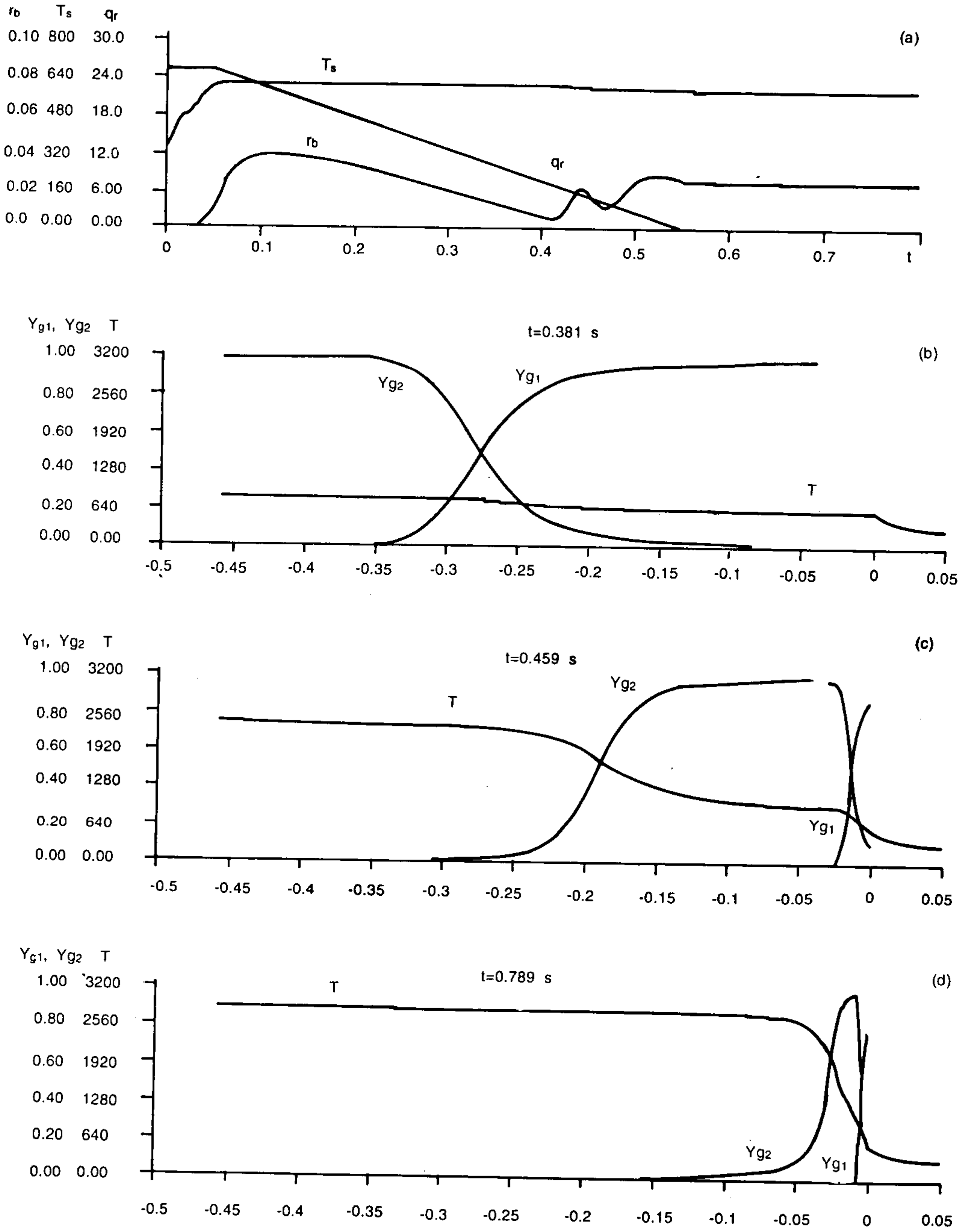

**Figure 4.** Three stage ignition ($q_o$ = 25 cal/cm$^2$s, $t_1$ = 0.05 s, $t_2$ = 0.55 s) (a), temporal distributions; (b), (c), and (d), spatial distributions ($t_b$ = 0.381 s, $t_c$ = 0.459 s, $t_d$ = 0.789 s).

self-sustaining combustion can be established if the time interval ($t_2$-$t_1$) is not much shorter than the characteristic relaxation time of preheat layer in this regime.

With relatively slow kinetics of the first gas phase reaction or high $q_o$, a two- stage regime is possible . The gas flame arises when the $T_s \approx T_b$ and evaporation starts. However, the flame is realized in the "zone separation regime", i.e. far from the surface at a distance $h \approx V_g t_{ign}$ Here $V_g \approx q_r$ is the velocity of gas issued from the surface and $t_{ign}$ is the induction time of thermal explosion in gas at characteristic temperature $Ts$. When $h >/(c_p V_g)$, the heat from the gas flame does not effectively feed to the surface. In this case, the gasification regime is observed presumably under action of the external heat flux $q_r$. When $q_r(t)$ decreases, the gas velocity and distance h also decrease and the flame approaches the surface. When $q_r$ vanishes, the flame provides the heat flux to the surface that is necessary for the steady-state self-sustaining regime (if deradiation was not too fast). In this case, the mass fraction of vapour above the surface $y_{ls}$, which in the zone separation regime of combustion coincides with $y_{cs}$, becomes less than $y_{cs}$ due to diffusion dilution of vapour by combustion products that leads to a small drop in $T_s$. As a result, the value (1-$y_{cs}$) decreases compared to gasification regime. It was obtained in numerical calculations performed for RDX-type EM.

With fairly "slow" kinetics of the second reaction in the gas phase (burning in the far zone) the three-stage regime is also possible (Fig. 4a). In this case, in the gasification regime, the gas flame of the first reaction is separated from the surface and heat feedback from gas is negligible (Fig. 4b). As $q_r$ decreases, the decomposition of the vapor becomes more intense and heat feedback to the surface increases. It leads to increase of temperature in gas layer near the surface. However, second reaction proceeds in a far zone and delivers very small part of heat to the surface (Fig. 4c). Finally, the flame in the far zone approaches the first flame and merges with it providing higher heat feedback to the surface (Fig. 4d).

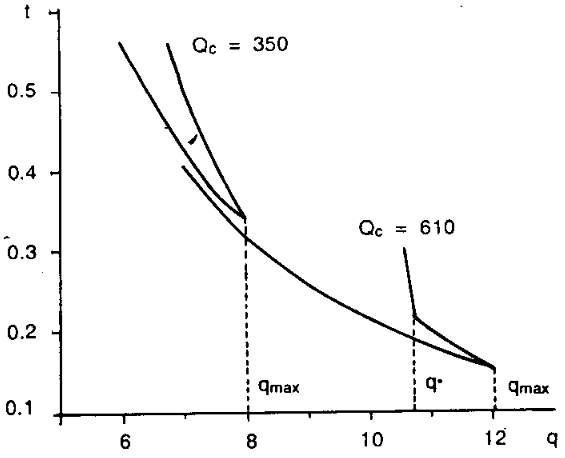

**Figure 5. Stability map for ignition transients.**

### 4.2 Stability of Combustion upon Deradiation

The problem of combustion stability under finite amplitude disturbance of combustion wave arises in case of ignition upon interrupted heating (in rocket motor it corresponds to the action of finite weight igniter) or in the case of transition from one steady-state regime to another under action of external factor. Use of deradiation makes it possible to study this problem in well characterized and experimentally reproducible conditions. The results of mathematical trials corresponding to well known experimental "go/no go" approach are shown in Fig. 5. The lower curve (Fig. 5) corresponds to a minimum exposure time which is needed to provide sustaining combustion of melted EM after deradiation.

According to the calculation data, with relatively low heat fluxes any overexposure of irradiated sample leads to transition to sustaining combustion. Starting from the critical value of external heat flux $q_*$ (simulation was made for opaque propellant) one may apply only short overexposure. The higher the heat flux, the shorter the allowable overexposure. Finally, there is a maximum critical value of heat flux $q_{max}$. With heat fluxes higher than $q_{max}$, a stable transition could not be achieved at any short duration of overexposure.

The values of $q_*$ and $y_{max}$ depend on kinetics and thermo-physical parameters of EM as well as on the deradiation rate. Obviously, the faster the deradiation, the closer are the values of $q_*$ and $q_{max}$.

## 5. DISCUSSION

A quantitative study of the combustion model for EM evaporated and decomposed in a condensed phase has revealed that at certain reference parameters of gas phase reactions, the ignition of EM may occur in three stages. Within the framework of the kinetic scheme used and with certain choice of parameters, the first initiation is caused by reaction in the condensed phase. However, an initiation of gas phase reactions requires a certain induction time which depends on kinetic coefficients. In particular, if the second reaction has a relatively slow kinetics, the final flame appears in a far zone and moves gradually to the surface.

Examination of the thermal and species profiles upon transient and stationary combustion regimes shows that for given melted-evaporated EM, a regime of condensed phase ignition (mainly due to exothermic decomposition in liquid subsurface layer) can be realised, followed by gas phase-controlled steady- state combustion (mainly due to heat feedback from gas phase reactions). This finding should be taken into account when one tries to use global kinetic parameters derived from the ignition tests for description of steady-state combustion of given EM.

It is known that the kinetic constants may be determined most reliably in experiments where a qualitative change in combustion behaviour is observed. Therefore, it is expected that comparison of the results of calculations and experiments on radiation driven combustion of EM with surface evaporation will allow one to reliably determine the unknown global kinetic constants of the gas phase reactions if, on varying the parameters of time-dependent radiant flux, the qualitative changes in the regression pattern (stage ignition, change of stage character) are obtained. The steady-state gasification regime realized in experiments may give valuable information about reaction kinetics in the liquid layer. It should be mentioned that the regime of flameless gasification under irradiation by NdYAG laser was experimentally observed in our laboratory with pressed samples of RDX and noncatalyzed double base propellant at atmospheric pressure.

The model developed gives excellent opportunities for theoretical study of transient combustion of evaporated EM. However, it has some limitations that should be carefully analyzed. One limitation concerns the mechanism of gas removal from subsurface melted layer. If the gases released beneath the burning surface form bubbles or jets, the structure of subsurface layer should be properly described in a comprehensive combustion model. Another limitation is the difficulty in simulating the combustion regimes with relatively weak heat feedback from the gas phase. There is experimental evidence for the existence of such combustion regimes for nitramines at elevated pressures[14] which, however, should be thoroughly checked in the future because of large scatter in and low reliability of temperature profile measurements at high burning rates

## 6. SUMMARY & CONCLUSION

In this work, a one-dimensional transient combustion model for melted and evaporated EM with exothermic reactions in condensed and gas phases has been developed. On the basis of the model, the effects of melting and exothermicity of condensed phase reaction on combustion stability have been studied. It has been established that the stability domain becomes broader when the melting temperature approaches the temperature of burning surface. The combustion of EM with remarkable exothermicity in condensed phase and weak heat feedback from gas flame has been shown to be intrinsically unstable. A transition from ignition to sustained combustion under careful deradiation can be effected, depending on kinetic parameters and the value of external heat flux, in one, two, or three stages. However, with fast deradiation, only low and moderate values of heat flux may provide successful transition to sustained combustion while, with high heat fluxes, such a transition is impossible in principle.

It is intended to continue work with the combustion model doing numerical experiments which simulate combustion of different types of EM with temperature-dependent properties. It is also intended to make improvements to the model by elaborating mechanisms of gas removal from subsurface melted layer and constructing a mechanism of heat transfer in this layer that allows stable combustion of EM with weak heat feedback from the gas flame.

## ACKNOWLEDGEMENT

The authors thank the European Research Office of the US Army for partial support of this study. The support and encouragement of Dr. Roy Reichenbach and Dr. Richard Miller of ONR are highly appreciated.

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