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SOME FUNDAMENTAL PROBLEMS ON THE
COMBUSTION OF LIQUID OXIDIZERS
IN HYDROGEN

BY

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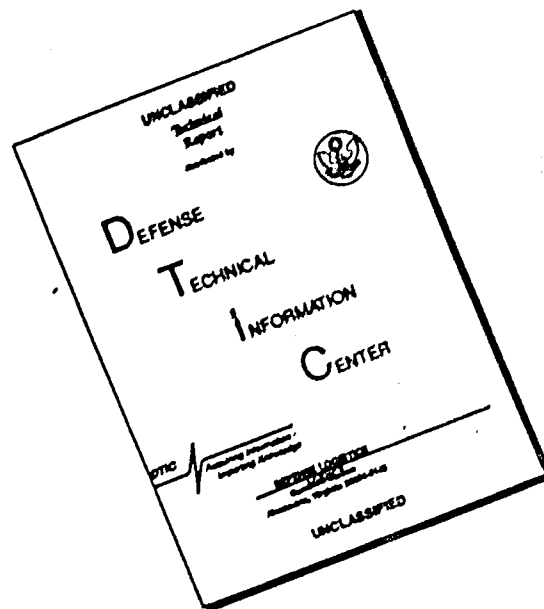
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I. INTRODUCTION.

Hydrogen is the most important high-energy fuel in rocket technology. Hydrogen-oxygen rocket motors are already being utilized, and other liquid propellant systems using hydrogen with several oxidizers are in a well advanced state of development.

Hydrogen has very distinctive physico-chemical characteristics. It has unusually low critical pressure of the order of 12 atmospheres with the result that it is injected into the combustion chambers of rocket motors at supercritical conditions. At pressures higher than the critical value the surface tension becomes equal to zero, and therefore hydrogen cannot form droplets within the combustion chamber, acting as a homogeneous fluid.

On the other hand, most oxidizers have critical pressures well above the normal working pressures of

liquid propellant rocket motors. Therefore, the basic combustion process in a rocket motor occurs as burning of a spray of oxidizer droplets within a hydrogen atmosphere.

The object of this paper is the study of the basic process of combustion of single oxidizer droplets in a quiescent hydrogen atmosphere.

There exists an abundant literature on droplet combustion (refs. 1,2,3 and 4, for example). Most studies refer to the case of fuel droplets burning in air. Some studies consider more sophisticated fuels and there are a few studies on monopropellant droplets.

On the other hand, no specific theoretical or experimental studies have been performed on the combustion of oxidizer droplets in hydrogen. This case cannot be included in a general theoretical study on droplet combustion owing to the specific properties of the hydrogen. Its low density and low molecular weight make diffusion conditions especially critical and the assumption of taking average values for gas density and for transport coefficients regardless of mixture composition, which is normally admitted in droplet combustion studies, may introduce important errors for the case of hydrogen and it is shown in the paper.

Some results on the combustion of nitric acid and bromine droplets in hydrogen were published by ourselves in Refs. 4 and 5. These studies have been completed and combustion of oxygen droplets has been also included .

Bromine was selected because chemical kinetics of the H_2-Br_2 reaction is well known, and this offered a good opportunity for the study of the influence of chemical kinetics on droplet combustion.

Nitric acid was chosen because this liquid oxidizer is particularly suitable to carry out experimental studies and, finally, oxygen was selected because of its high technical interest. This last study is an application of a general study on the hydrogen-oxygen diffusion flame with spherical symmetry, shown in Refs. 6 and 7.

2 - MODEL OF THE PROCESS

Combustion of oxidizer droplets in hydrogen atmosphere will be studied under the following assumptions :

- 1 - Spherical Symmetry. Therefore, natural convection effects, always small in a hydrogen atmosphere, will be disregarded.
- 2 - Stationary conditions. Recession velocity of the droplet surface will be disregarded as compared with

diffusion velocities of chemical species, and the energy and time required to heat up the droplet up to its boiling temperature will be also disregarded.

- 3 - Constant pressure since it is practically constant in this type of processes.
- 4 - Three chemical species: Hydrogen, oxidizer and reaction products will only be considered. The influence of radicals will only appear through the chemical kinetics of the process.
- 5 - An over-all reaction rate will be taken in order to consider chemical kinetics of the process. This over-all reaction rate may be derived from the complete chemical reaction model of the combustion process.
- 6 - A linear variation of gas density and thermal conductivity as function of mixture composition will be considered.

3 - FUNDAMENTAL EQUATIONS

The fundamental equations of the process will be expressed in terms of the dimensionless variables :

$$x = \frac{C^0}{M_1} \quad \frac{1}{4 \pi \bar{\lambda}} \quad \frac{\dot{m}}{r} \quad (1)$$

$$\theta = -\frac{C_p^o}{q_r} (T - T_o) \quad (2)$$

and the over-all combustion reaction will be assumed to be of the form :

$$\nu_1 M_1 + \nu_2 M_2 = \nu_3 M_3 \quad (3)$$

Under the aforementioned assumption and in terms of x and θ the fundamental equations of the process are as follows:

a) Continuity

$$\frac{d \mathcal{E}_1}{dx} = -\frac{C_p^o}{M_1 \lambda} \frac{x^2}{x^4} \frac{r_s^2}{r_s^4} w_1 \quad (4)$$

which expresses the conservation of mass of each chemical species 1 .

b) Energy

$$\begin{aligned} (\mathcal{E}_1 - 1) \frac{\nu_3}{\nu_1} + \theta \left[1 + \frac{\nu_1 + \nu_2 - \nu_3}{\nu_1} (\mathcal{E}_1 - 1) \right] + \\ + \frac{\lambda}{\lambda} \frac{d\theta}{dx} + \theta_o = 0 \end{aligned} \quad (5)$$

This equation expresses that the sum of the energy fluxes of heat and enthalpy is constant. This constant has been obtained by expressing at the droplet's surface that

the heat received by the droplet is utilized in evaporating the liquid.

In this equation parameter Θ_o is :

$$\Theta_o = \frac{q_1^o}{q_r^o} + \frac{C_p^o (T_s - T_o)}{q_r^o} \quad (6)$$

Standard heat of reaction q_r^o is given by :

$$q_r^o = \frac{1}{\nu_j} (\nu_1 h_{1,o}^o + \nu_2 h_{2,o}^o - \nu_3 h_{3,o}^o) \quad (7)$$

c) Diffusion

Assuming that only concentration diffusion exists, it results :

$$\sum_j \left[\frac{Y_j}{M_j} \frac{\bar{f}_{ij}}{\rho} \mathcal{L}_{ij} + \frac{1}{Y_i} \frac{d Y_i}{dx} - \frac{1}{Y_j} \frac{d Y_j}{dx} \right] = 0 \quad (8)$$

in which, $\mathcal{L}_{ij}$ is the Lewis-Semenov number given by :

$$\mathcal{L}_{ij} = \frac{M_1}{C_p^o} \frac{\bar{\lambda}}{\bar{f}_{ij} D_{ij}} \quad (9)$$

d) Boundary Conditions

Boundary conditions are as follows :

At the droplet's surface :

$$x = x_s \quad \left\{ \begin{array}{l} \theta = \theta_s \\ \epsilon_{1s} = 1 ; \epsilon_{2s} = \epsilon_{3s} = 0 \end{array} \right. \quad (10)$$

At the infinity :

$$x = 0 \quad \left\{ \begin{array}{l} \theta = \theta_\infty \\ Y_{1\infty} = 0 \quad \epsilon_{1\infty} = 0 \\ Y_2 = Y_{2\infty} , Y_3 = Y_{3\infty} \end{array} \right. \quad (11)$$

4 - SOLUTION OF THE SYSTEM

In the first place the problem will be solved by assuming an infinitely fast reaction rate, which is equivalent of taking a zero-thickness reaction zone.

This is the well known Burke and Schumann assumption for studying flames and it has been proven⁴ that it gives a good approximation of results in droplet combustion provided that the droplets are not too small or the pressure is not too low.

In this case in which hydrogen is the reactant atmosphere with a molecular weight much smaller than that of the oxidizer droplet, it was considered that the influence of mixture composition on the value of density and thermal conductivity

might be specially important. Therefore, linear variations of density and thermal conductivity as functions of mass fraction of the combustion products were taken:

$$\frac{\rho}{\rho_{1j}} = a_{13} + b_{13} Y_3 \quad (12)$$

$$\frac{\lambda}{\lambda} = c_{13} + g_{13} Y_3 \quad (13)$$

With the Burke-Schumann assumption, the problem has an exact analytical solution.

Mass fraction and temperature are given by :

Zone $0 \leq x \leq x^0$

$$\frac{\epsilon_{3\infty} - Y_{3\infty}}{\epsilon_{3\infty} - Y_3} = \exp \left[\frac{\mathcal{L}_{23} x - b_{23} (Y_{3\infty} - Y_3)}{b_{23} \epsilon_{3\infty} + a_{23}} \right] \quad (14)$$

$$\left[\frac{\nu_2 - \nu_1 \theta_0 - (\nu_2 - \nu_1) \theta}{\nu_3 - \nu_1 \theta_0 - (\nu_3 - \nu_2) \theta_{\infty}} \right]^{\nu_1 / \nu_3 - \nu_2} = \frac{a_{23} + b_{23} \epsilon_{3\infty}}{\mathcal{L}_{23} (c_{23} + g_{23} \epsilon_{3\infty})} \times \left[\frac{\epsilon_{3\infty} - Y_{3\infty}}{\epsilon_{3\infty} - Y_3} \cdot \frac{c_{23} + g_{23} Y_{3\infty}}{c_{23} + g_{23} Y_3} \right]$$

$$\times \left[\frac{c_{23} + g_{23} Y_3}{c_{23} + g_{23} Y_{3\infty}} \right]^{b_{23} / g_{23} \mathcal{L}_{23}} \quad (15)$$

Zone $x \ll x^* \ll x_s$

$$\frac{Y_{3s}}{Y_3} = \exp \left[\frac{\alpha_{13}(x - x_s) - b_{13}(Y_{3s} - Y_3)}{a_{13}} \right] \quad (16)$$

$$\frac{\theta + \theta_0}{\theta_s + \theta_0} = \left[\frac{Y_3}{Y_{3s}} \right]^{\frac{a_{13}}{c_{13} \alpha_{13}}} \cdot \left[\frac{c_{13} + g_{13} Y_3}{c_{13} + g_{13} Y_{3s}} \right]^{\frac{b_{13}}{g_{13} \alpha_{13}}} - \frac{a_{13}}{c_{13} \alpha_{13}} \quad (17)$$

Dimensionless burning rate x_s :

$$x_s = \frac{C_p^0}{M_1} \frac{1}{4 \pi \lambda} \frac{\dot{m}}{r_s} \quad (18)$$

is obtained by expressing in the foregoing equations that for $x = x_s$ is $\theta = \theta_s$.

Flame front position $x = x^*$ and maximum temperature θ^* are obtained by expressing that for $x = x^*$ is $Y_3 = 1$

From the value of x_s the evaporation constant k , equal to the slope of curve $r_s^2 = f(t)$ is obtained by

means of the expression :

$$k = - \frac{dr^2}{dt} = - \frac{\dot{m}}{4 \pi \rho_1} \quad (19)$$

5 - THEORETICAL RESULTS FOR INFINITE REACTION RATE

Theoretical results of the dimensionless burning rate x_b , evaporation constant k and flame/droplet radius ratio $r^{\bullet}/r_m$ were obtained for nitric acid, bromine and oxygen droplets assuming an infinitely fast reaction rate.

Results are shown in Table No. 1, in which, for comparison, results corresponding to the combustion of hydrocarbons droplets in air are also included, as well as some other representative propellant combinations.

It may be seen that combustion in hydrogen is considerably faster and that the flame is much closer to the droplet surface than in the other propellant combinations .

It is also shown in the Table the very important influence, for the case of combustion of oxygen droplets in hydrogen, of considering constant or variables values of the gas density and transport coefficients as function of mixture composition.

6 - FINITE REACTION RATE

System of differential equations (4), (5) and (6) was solved for the case of finite reaction rate by utilizing the approximated analytical method described in Refs. 4 and 5 .

For applying this analytical method an over-all reaction rate is needed. Therefore, it could not be utilized for the cases of nitric acid and oxygen for which such over-all reaction rates were not available.

For the bromine-hydrogen reaction the Campbell and Hirschfelder reaction model was adopted from which an over-all reaction rate was obtained (see Ref. 5).

Results were obtained as function of the dimensionless product of the $3/4$ th power of the pressure multiplied by the droplet radius in the form :

$$x_s = \varphi(Q^{1/2} p^{3/4} r_s) \quad (20)$$

$$x \frac{\frac{x_s}{x^\bullet}}{\frac{r_s}{r^\bullet}} = \psi(Q^{1/2} p^{3/4} r_s) \quad (21)$$

in which parameter Q is given by:

$$Q = 1.8816 \cdot 10^9 M_3 (M_2/M_1)^{1/2} (RT_f)^{-3/2} \bar{c}_p \bar{\lambda}^{-1} \quad (22)$$

The values of x_s and $r^{\bullet}/r_s$ are shown in Figs. 1 and 2 in which the values for nitric acid and oxygen droplets for the case of an infinitely fast reaction rate are also shown.

Results show that for the case of bromine droplets combustion does not exist under a minimum value of either the pressure or the droplet radius[•]. It may also be seen that above this value results tend rapidly towards those obtained assuming an infinitely fast reaction rate.

7 - EXPERIMENTAL RESULTS

Experimental results were obtained by burning droplets suspended of a thin quartz fiber in a chamber filled with hydrogen at different pressures. Photographic records were taken of the droplets diameter and flame diameter as function of time

 •.- This conclusion was established in general for droplets combustion considering finite chemical kinetics in Ref. 4 .

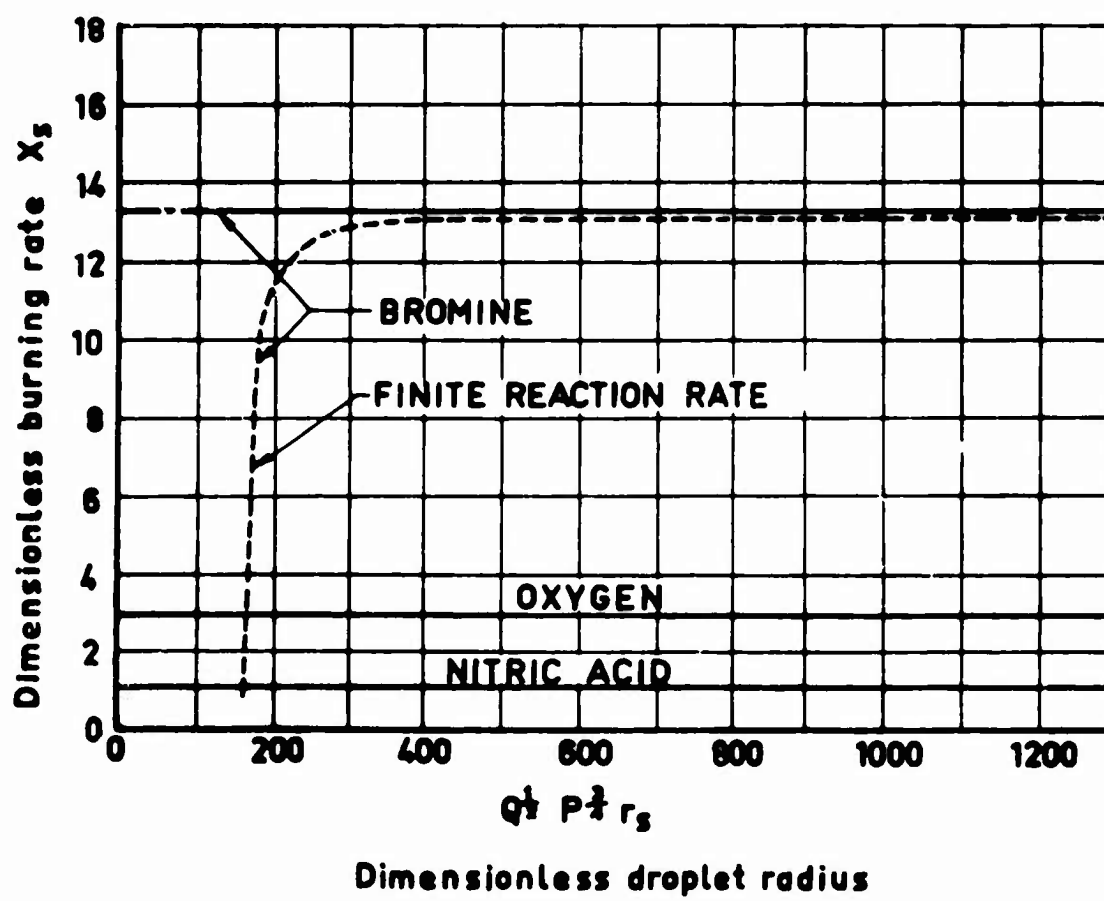


FIG. 1

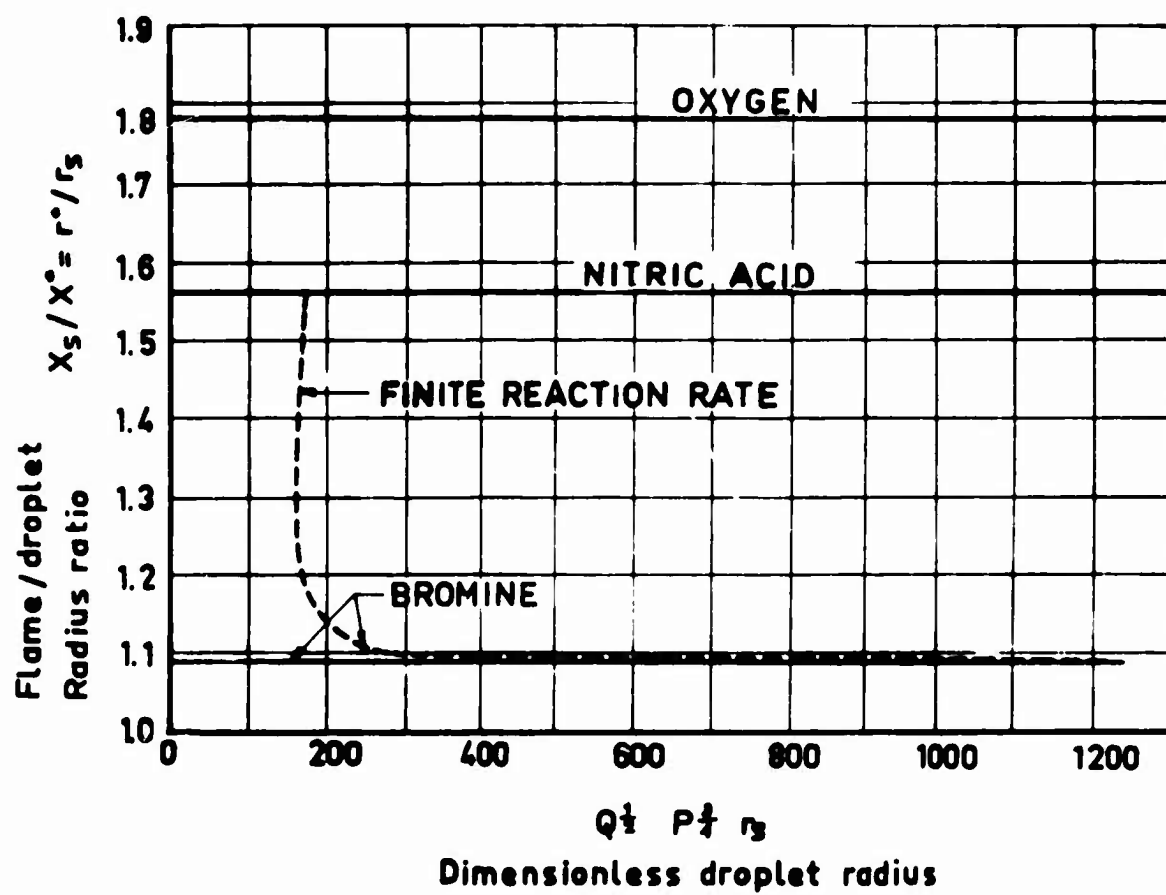


FIG. 2

These experimental studies were only carried out for nitric acid and bromine droplets since it was not possible to carry out this experimental work for oxygen droplets.

Experimental results for nitric acid droplets are shown in Fig. 3, and numerical results obtained in Table No. 1, in which it may be seen that there is a reasonable agreement between theoretical and experimental results.

Combustion of bromine droplets in hydrogen is of an explosive type, as high-speed photographs show in Fig. 4. A similar type of combustion has been observed sometimes in metal particles and there not yet exists a clear understanding of this phenomenon.

Due to this type of rough combustion comparison between theoretical and experimental results was not, for this case, carried out.

8 - CONCLUSIONS

a) Combustion of liquid oxidizers in hydrogen occurs as burning of a spray of oxidizers droplets in an homogeneous hydrogen atmosphere.

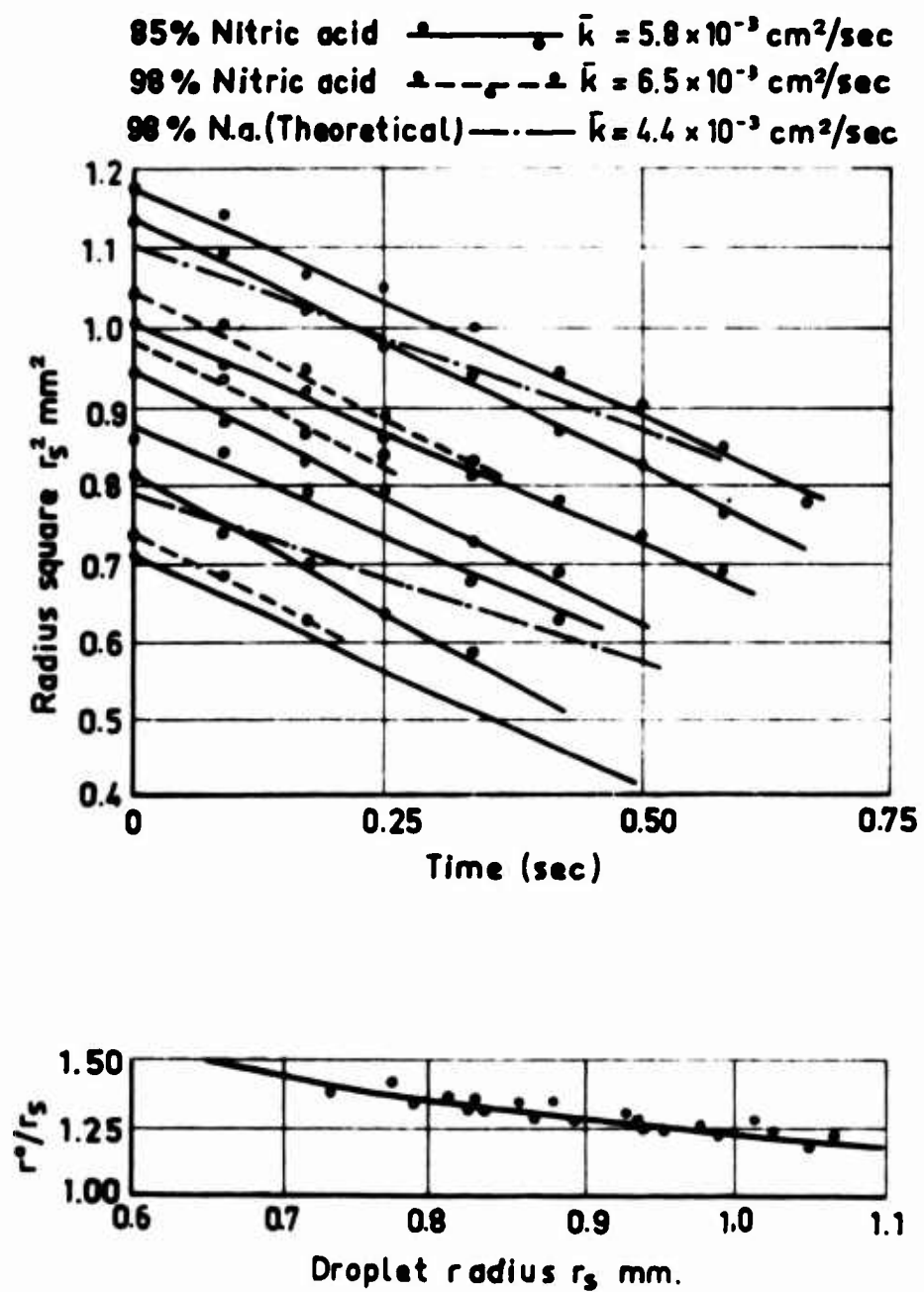


FIG. 3

T A B L E No. 1

BURNING RATES, EVAPORATION CONSTANTS AND FLAME-DROPLET

RADIUS RATIO

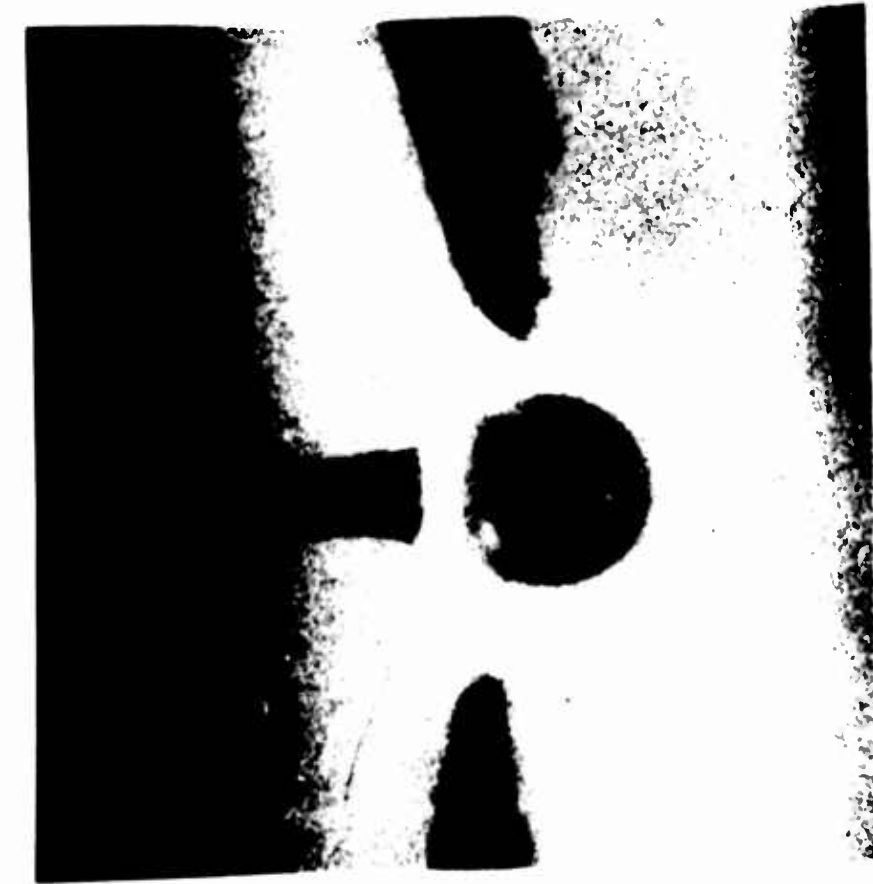
	Dimensionless burning rate $x_s \sim -\frac{\dot{m}}{r_s}$	Evaporation constant $k \sim -\frac{dr_s}{dt}$, $\text{cm}^2/\text{sec.}$	Flame/droplet radius ratio r^*/r_s
Oxygen droplets in hydrogen (constant transport coefficients)	4.00	3.27×10^{-3}	2.10
Oxygen droplets in hydrogen (variable transport coefficients)	2.80	5.79×10^{-3}	1.78
Nitric acid droplets in hydrogen (theoretical)	1.02	4.4×10^{-3}	1.53
Nitric acid droplets in hydrogen (experimental)	---	6.5×10^{-3}	1.30 (average)
Bromine droplets in hydrogen (theoretical)	13.2	12.6×10^{-3}	1.095
N-heptane in air (experimental)	---	$2.73 \times 10^{-3}^\bullet$	3.10
Benzene in air (experimental)	---	$2.50^\bullet$	3.0
Ethyl Alcohol in air (experimental)	---	$1.98^\bullet$	3.5
Hydrazine in nitrogen (experimental, $T_\infty = 520^\circ\text{C}$)	---	$1.70 \times 10^{-3}^\bullet$	$\approx 6.0^\bullet$
Hydrazine in nitrogen (experimental, $T_\infty = 700^\circ\text{C}$)	---	$2.70^\bullet$	$\approx 5.0^\bullet$

•.- Data taken from our own experimental results.

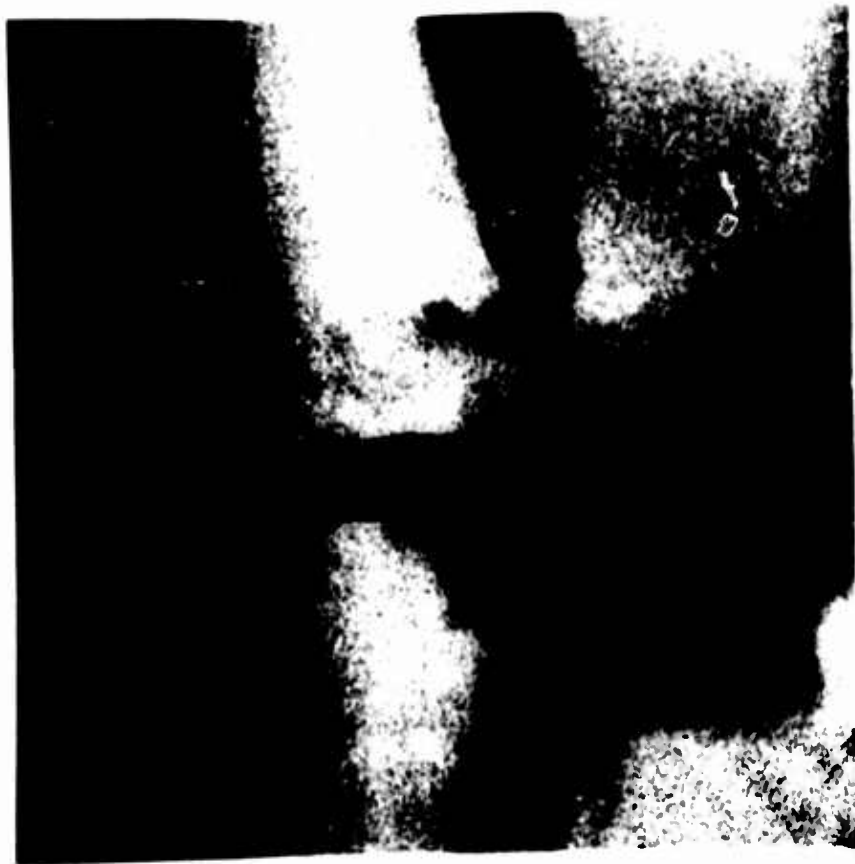
b) Combustion of oxidizer droplets in hydrogen is much faster than combustion of most usual combinations of propellants.

c) The hydrogen-oxidizer flame is located very close to the oxidizer droplet surface.

d) When calculating combustion of liquid oxidizers in hydrogen it is important to take into account proper values of gas density and transport coefficients as function of mixture composition.



Ignition, $t = 0$



Explosive Combustion,

$t = 1,500$ sec.

Fig. 3 A bromine droplet burning in hydrogen

$P = 5.5$ atm.

LIST OF PRINCIPAL SYMBOLS

- C_p^0 - molecular heat capacity at constant pressure (constant).
 D_{ij} - diffusion coefficient
 $\dot{m}$ - mass flow.
 M - molecular weight
 p - pressure
 q_1^0 - molar heat of evaporation of liquid oxidizer
 q_r^0 - molar heat of reaction
 r - radius
 w_1 - reaction rate.
 x - dimensionless coordinate
 Y_1 - mass fraction of species 1
 $\mathcal{E}_1$ - flux fraction of species 1
 $\bar{\lambda}$ - average value of thermal conductivity
 ν - stoichiometric coefficients.
 $\bar{\rho}_{ij}$ - average value of density of species i and j.
 θ - dimensionless temperature

Subscripts

- 1,2,3 - oxidizer, hydrogen and reaction products, respectively.
 s - at the droplet surface.

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