DIFFUSION FLAMES AND SUPersonic COMBustion

BY

I. DA-RIVA A. LIÑAN
E. FRAGA J. L. URRUTIA

INSTITUTO NACIONAL DE TECNICA AEREOspacial
"ESTEBAN TERRADAS"
MADRID (SPAIN)
October 1, 1967
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABSTRACT</td>
<td>1</td>
</tr>
<tr>
<td>NOMENCLATURE</td>
<td>3</td>
</tr>
<tr>
<td>I. INTRODUCTION</td>
<td>5</td>
</tr>
<tr>
<td>II. HYDROGEN-AIR FREE SHEAR LAYER</td>
<td>8</td>
</tr>
<tr>
<td>2.1 Hydrogen-Air Chemical Kinetics</td>
<td>8</td>
</tr>
<tr>
<td>2.2 Simplified Formulation of the Mixing Problem</td>
<td>12</td>
</tr>
<tr>
<td>III. IGNITION DELAY ZONE</td>
<td>17</td>
</tr>
<tr>
<td>3.1 The Distribution of Hydrogen Atoms in the Ignition Delay Zone</td>
<td>17</td>
</tr>
<tr>
<td>3.2 The Initial Concentration of Atomic Oxygen</td>
<td>27</td>
</tr>
<tr>
<td>3.3 The Ignition Delay Zone Length</td>
<td>33</td>
</tr>
<tr>
<td>IV. AERODYNAMIC FIELD NEAR THE INJECTOR EXIT</td>
<td>38</td>
</tr>
<tr>
<td>4.1 Flow Configuration at Low Injection Rates</td>
<td>38</td>
</tr>
<tr>
<td>DISCUSSION</td>
<td>44</td>
</tr>
<tr>
<td>CONCLUSIONS</td>
<td>45</td>
</tr>
<tr>
<td>POSSIBLE RELATED EFFORTS</td>
<td>46</td>
</tr>
<tr>
<td>REFERENCES</td>
<td>47</td>
</tr>
</tbody>
</table>
ABSTRACT

Some problems related to the fluid dynamical and chemical phenomena appearing near the injector exit of an idealized supersonic combustion burner, are theoretically investigated.

When hydrogen is injected into a coflowing supersonic stream of air, a wake-like configuration appears in most cases, improving the mixing process.

It is only natural to suggest that whenever the ignition delay length, computed assuming isobaric mixing and reaction, is not much larger than the recirculation zone length, the wake will influence the ignition zone.

In order to calculate the ignition delay length, the usual assumption is made that fuel and oxidizer mix without appreciable concentration change and heat release resulting from chemical reactions, although radicals, mainly atomic hydrogen, are produced. The chemical kinetics scheme is reduced to one overall chemical reaction; and the presence of radicals introduced in the mixing zone from outside is taken into account. A two-dimensional mixing zone has been considered.

Although many different mechanisms will be responsible for the fortuitous or provoked production of these radicals either in real flight or in ground testing facilities, dissociation at the injector outer boundary layer is considered in this paper as the main radicals producing mechanism.

As it is shown, the temperature of the injector outer wall and, to a less extent, pressure, injector length and the conditions outside of the boundary layer, control the amount of radicals introduced in the mixing layer, and hence the ignition delay length.
Finally, it is shown that ignition delay lengths are, in most cases of interest, comparable to the near-wake length.

The paper ends with a discussion of the main weaknesses of the work presented and with some suggestions for further work.
NOMENCLATURE

\( E_j \) = activation energy of reaction \( j \)
\( f_1, f_2 \) = defined by Eq. (6)
\( I \) = flux of atomic oxygen across the injector boundary layer at the injector exit
\( k_j \) = rate constant of reaction \( j \)
\( K_j \) = rate of reaction \( j \)
\( l \) = injector length
\( m_i \) = molecular weight of species \( i \)
\( M \) = Mach number
\( N \) = defined by Eq. (8)
\( P \) = pressure
\( r \) = injector radius
\( R \) = universal gas constant
\( T \) = temperature
\( u, v \) = velocity components along the \( x, y \) coordinates
\( U \) = \( \frac{1}{2} (u_o + u_r) \)
\( w_j \) = mass production rate per unit volume of species \( j \)
\( x, y \) = intrinsic system of coordinates, see Fig. 2
\( x_n \) = defined by Eq. (12)
\( Y_2 \) = mass fraction of \( H_2 \)
\( Y_3 \) = \( O_2 \)
\( Y_5 \) = \( H \)
\( Y_6 \) = \( O \)
\( Z_n \) = defined by Eq. (14)
\( \varepsilon \) = non-uniformity factor introduced in Eq. (8)

\( \varepsilon \) = turbulent diffusivity

\( \lambda \) = \( \frac{u_p}{u_0} \) fuel to air velocity ratio

\( \xi, \eta \) = similarity variables

\( \rho \) = density

\( \sigma \) = Görtler's similarity parameter

\( \tau \) = ignition delay time

**Subscripts**

\( o \) = undisturbed air stream conditions

\( F \) = undisturbed fuel stream conditions
I. INTRODUCTION

In recent years considerable attention has been devoted to the study of supersonic combustion in order to develop a hyper-sonic air-breathing vehicle in which the entering stream would be slightly decelerated, so that large increases of static temperature and losses associated with the air deceleration are avoided. In the combustion system of such a vehicle the very rapid mixing and burning of fuel in the air stream is intended. The propulsion system using this form of combustion is called SCRAMJET (Supersonic Combustion Ramjet).

It appears that SCRAMJET propulsion would make it possible to place heavy loads in orbit, by powering the atmospheric stage with this form of propulsion and using lighter, smaller, and more maneuverable vehicles than would be feasible with rocket propulsion. Furthermore, present results show that direct operating costs for ramjet powered hypersonic airplanes would not be greater than for the supersonic transport.

Among all the proposed systems of supersonic combustion, the purely diffusive mode is the one which fits better to the large flight Mach numbers (6 ≤ M ≤ 25), since a small deceleration of the flow may be enough to increase the pressure and temperature, so that fuel and oxidizer burn as soon as they reach the reaction zone.

Diffusive supersonic combustion presents very challenging basic problems, due to the incomplete state of knowledge in some related areas such as chemical kinetics and turbulent mixing of gases, especially gases of very different densities.

A simple model of the supersonic combustion system would consist of a hydrogen jet injecting downstream into a faster co-
flowing air stream, Fig.1. For analytical purposes three different operating regions can be considered.

a) Near-equilibrium diffusion flame. The characteristic chemical time for the chemical reaction to take place is much smaller than the mixing time. The chemical reaction takes place in a very thin region whose location is controlled by the mixing process.

b) Near frozen mixing. The characteristic chemical time is much higher than the mixing time. The chain initiation reactions are very slow, so that fuel and oxidizer mix without either appreciable concentration change or heat release resulting from the chemical reactions. Nevertheless radicals, mainly H, are produced.

c) Intermediate or Transition region where both characteristic times are similar.

This paper deals with the analytical study of the chemical and fluid dynamical phenomena appearing near the injector exit in a supersonic combustion burner.

The main features of these phenomena are:

a) From the chemical point of view the fact that being the temperature low, near frozen mixing conditions prevail.

b) From the fluid-dynamical point of view the fact that when hydrogen is injected parallel to a supersonic air stream, a wake like configuration appears in most cases, improving the mixing process.

The paper is organized in the following form. First the problem of the near frozen mixing in a two-dimensional free mixing layer which separates two parallel streams of hydrogen and
air is considered. The chemical kinetics of the process is studied using an overall chemical reaction, together with the assumption that fuel and oxidizer mix without appreciable concentration change and heat release resulting from chemical reactions. Special emphasis is placed on discerning the initiation reaction. It is shown that in many cases, dissociation in the injector outer boundary layer is the main triggering mechanism.

The fluid-dynamical pattern is studied by linearizing the mixing problem, following essentially the approach taken to study the turbulent jet mixing between two streams at constant pressure by some authors. Under such simplifications the study is relatively simple and may be easily extended to more complex flow fields.

The goal of this part of the paper is to calculate the ignition delay distance measured along the center line of the free shear layer. It is shown that under some circumstances, the resulting ignition delay lengths are comparable to those measured in premixed hydrogen-air mixtures.

The next step is to compare this distance with the recirculation length of the wake-like configuration which appears near the injector exit. Low injection velocities favour the recirculating wake configuration and provide rapid mixing but increase the jet area and the geometrical scale of the flow pattern.

II. HYDROGEN-AIR FREE SHEAR LAYER

2.1 Hydrogen-Air Chemical Kinetics

The analysis of the ignition delay in Hydrogen-Air systems has been the subject of many theoretical and experimental investigations. A recent exposition of this topic, containing a fairly comprehensive bibliography is presented in 1.
The models used to study the kinetics of the Hydrogen-Air systems involve a given number of chemical kinetic equations (from nine to twenty depending on the pressure and temperature ranges considered).

The temperature of the incoming air stream is, in the cases of interest to supersonic burners, of the order of 1300°K, and the pressure of one atmosphere. Lower temperatures and pressures would give rise to larger ignition delays. On the other hand, if the air static temperature at the injector exit were much larger than the above mentioned value, the final combustion temperature would be too high and the products would leave the combustor with a large amount of dissociation.

For these temperatures and pressures, the chemical kinetic scheme is reduced to the following elementary processes

\[
\begin{align*}
0 & : \quad H_2 + O_2 \rightarrow 2OH \\
1 & : \quad OH + H_2 \rightarrow H_2O + H \\
2 & : \quad H + O_2 \rightarrow OH + O \\
3 & : \quad O + H_2 \rightarrow OH + H
\end{align*}
\]

The role played by the remaining reactions of the more complete kinetics is purely marginal owing to their small specific reaction rates, and the low concentration of intermediate and final species involved. In particular Nitrogen is treated as an inert diluent.

Writing the rate constants of the significant reactions in the form

\[ K_j = k_j e^{-E_j/RT} , \]

we condense the pertinent values in Table 1.
TABLE 1 - RATE CONSTANTS.

<table>
<thead>
<tr>
<th>j</th>
<th>$k_j$</th>
<th>$E_j$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$10^{14}$</td>
<td>$7 \times 10^4$</td>
</tr>
<tr>
<td>1</td>
<td>$3 \times 10^{14}$</td>
<td>$6 \times 10^3$</td>
</tr>
<tr>
<td>-1</td>
<td>$1.2 \times 10^{15}$</td>
<td>$2.06 \times 10^4$</td>
</tr>
<tr>
<td>2</td>
<td>$3 \times 10^{14}$</td>
<td>$1.75 \times 10^4$</td>
</tr>
<tr>
<td>3</td>
<td>$3 \times 10^{14}$</td>
<td>$8 \times 10^3$</td>
</tr>
</tbody>
</table>

The temperature $T$ is in °K, the rate constants in (mole/cc)$^{-1}$ sec$^{-1}$, and the activation energies $E_j$ in cal/mole °K.

Subscript $-j$ denotes reverse $j$ reaction. Reaction $-1$ will be used in order to give a criterium to define the end of the ignition delay zone.

The rate constant of the chain initiation reaction 0 is very small, so that this reaction is responsible for the large ignition delays appearing in the hydrogen-oxygen combustion processes. When there is an appreciable amount of radicals, $\text{H}$, $\text{OH}$ or $\text{O}$, initially present either in the air or in the fuel streams, the initiating reaction may become unimportant; otherwise it is the only initiation mechanism occurring in practice under conditions relevant to supersonic combustion studies.

In addition, the forward rate constants of reactions 1 and 3 are larger than the constant corresponding to the forward reaction 2. Hence we may assume, following $^2$, that in most of the ignition delay region:

1st. Any amount of 0 initially present will be converted, by means of the fast reaction 3, into $\text{OH}$ and $\text{H}$.
Similarly, any OH initially present or produced by the reactions 0 or 3, will be immediately depleted by the reaction 1, producing H$_2$O and H.

3rd. The OH atoms produced by the relatively slow reaction 2, will be soon converted into H and H$_2$O by means of the reactions 1 and 3.

Summarizing, if for any reason (such as dissociation in the injector outer boundary layer) some concentration of atomic oxygen is initially present near the injector exit, we may assume that each atom of oxygen reacts immediately with two molecules of H$_2$ producing two atoms of H and one molecule of H$_2$O. Similarly, each mole of OH gives rise to one mole of H and one mole of H$_2$O. Hence, the set of processes 0, 1, 2 and 3 may be substituted by the over-all reaction

$$3H_2 + O_2 \rightarrow 2H_2O + 2H,$$

obtained combining 0, 1, 2 and 3 in such a way that neither O nor OH appear as reactant or product.

In the case of Hydrogen-Air premixed systems, it has already been shown that the transition time between the radicals producing reactions and the action of the chain (reactions 1, 2, 3) is a small fraction of the ignition delay time.

The over-all production rate of H is:

$$\frac{w_5}{m_5} = \frac{w_1}{m_1} = 2K_0 \rho^2 \frac{Y_2}{m_2} \frac{Y_3}{m_3} + 2K_2 \rho^2 \frac{Y_3}{m_3} \frac{Y_5}{m_5}.$$ (1)

Once a sufficient number of hydrogen atoms has been produced, the various reactions occur rapidly and exothermally so that the temperature begins to increase and the concentration of
the main reacting species $H_2$ and $O_2$ begin to decrease. However, the structure and boundaries of the ignition delay region may be determined assuming, as a first order approximation, that fuel and oxidizer mix without concentration change and heat release resulting from the chemical reaction.

There are many criteria to define the end of the ignition zone. One could use as a criterium that the reverse reaction 1 should be of the same order as the forward reaction 2. Afterwards the amount of $OH$ and $O$ would grow rapidly until a partial equilibrium is attained.

2.2 Simplified Formulation of the Mixing Problem

A considerable amount of effort has been devoted in the past to the study of jet mixing. Our analysis of the turbulent free mixing layer between two streams, follows essentially the approach advanced earlier by Korst et al. to deal with the mixing between one stream and the quiescent fluid.

Although the problem of turbulent mixing of gases is far from settled (too many obscure points remain when the simple Korst model is applied to the mixing of a very high Mach number airstream with a so dissimilar gas as hydrogen) the main advantage of this treatment lies in the fact that, while retaining some peculiarities of the real phenomena, it may be extended to more complex flow fields such as the wake and cavity flows.

In the case considered, of low speed parallel hydrogen injection in a supersonic stream, the mass and momentum injection rates are very low, so that it seems logical to assume that this injection does not appreciably disturb the wake-like configuration, and a treatment similar to that considered by Korst may be used to describe the fluid dynamic aspects of the problem. Such a treatment takes into account the following phenomena:
a) expansion around the injector exit, b) turbulent mixing at constant pressure along the wake boundaries, c) pressure rise at the neck, and d) mass conservation inside the wake.

In the present section we are particularly concerned with the isobaric mixing mechanism between two uniform, parallel streams. The results may be useful to study part b) in the Korst model.

We may write the equation of motion in the following form:

$$ u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = \varepsilon \frac{\partial^2 u}{\partial y^2} \quad (2) $$

where $\varepsilon$ is the (apparent) eddy diffusivity for the turbulent flow.

In the analysis by Korst, a linearized equation of motion is solved, resulting in the velocity profile equation

$$ u = \frac{u_o + u_F}{2} + \frac{u_o - u_F}{2} \operatorname{erf} \eta \quad (3) $$

where

$$ \eta = \frac{y}{2} \int x \frac{\varepsilon}{\nu} \, dx $$

$$ U = \frac{1}{2} (u_o + u_F) $$

$u_o$, $u_F$ = undisturbed velocities in either side of the free mixing zone

$$ \operatorname{erf} \eta = \frac{2}{\sqrt{\pi}} \int_0^\eta e^{-\beta^2} \, d\beta $$

Because of the many simplifications in the equation of motion, the velocity and temperature fields are interpreted to hold in an intrinsic system of coordinates $(x,y)$, shifted in the
Y direction from the physical coordinates \((X, Y)\) accordingly

\[
x = X
\]

\[
y = Y + y_m(x)
\]

where \(y_m(0) = 0\) (Fig. 2).

The orientation of the intrinsic system of coordinates with respect to the physical system is accomplished by using a momentum integral equation.

The effect of the injector boundary layers on the velocity profiles in the free shear layer has been neglected, otherwise Eq. (3) is not valid very near the injector exit.

Consistently with this approximation, the equations of conservation of species are written in the following form:

\[
\frac{\partial^2 Y_i}{\partial \eta^2} + 2\eta \frac{\partial Y_i}{\partial \eta} = - \left[ \frac{u}{\varepsilon} \int \frac{e}{U} \, dx \right] \left[ \frac{w_i}{\rho} - U \frac{\partial Y_i}{\partial x} \right], \quad (4)
\]

where, as in the momentum equation, it has been assumed that \(v\) is negligible and \(u\) can be approximated by \(U = (u_0 + u_p)/2\) in the sense of Pai's small perturbation concept.

Since we are dealing with the region close to the injector exit, we may assume that the expression

\[
\varepsilon(x) = \varepsilon_\infty x
\]

is to hold, where \(\varepsilon(x)\) and \(\varepsilon_\infty\) are average values across the mixing region.

Eq. (4) becomes:
$T_F = 1000^\circ K$

$u_0 = 3000 \text{ m/sec}$

$T_o = 1300^\circ K$

$\lambda = 0.4$

$T_o = 1600^\circ K$

$\lambda = 0.8$

FIG. 3 - FACTOR OF REACTION 2 vs $\eta$
The temperature may be determined in terms of the total enthalpy using the Crocco integral, since frozen mixing conditions prevail.

III. IGNITION DELAY ZONE

3.1 The Distribution of Hydrogen Atoms in the Ignition Delay Zone

In calculating the distribution of hydrogen atoms throughout this zone, we will make use of the simplifications mentioned in the two foregoing paragraphs.

If we insert Eq. (1) into Eq. (5) we are led to the following linear differential equation:

\[
\frac{\partial^2 Y_5}{\partial \eta^2} + 2n \frac{\partial Y_5}{\partial \xi} - 2 \xi \frac{\partial Y_5}{\partial \xi} + 2 \xi f_1(\eta)Y_5 = -2 \xi f_2(\eta),
\]

where

\[
f_1(\eta) = \frac{K_2^\rho \frac{-Y_3}{m_3m_5}}{\left(K_2^\rho \frac{Y_3}{m_3m_5}\right)_0}
\]

and
FIG. 4 - FACTOR OF REACTION $\phi$ vs $n$

$T_F = 1000^\circ$K
$\lambda = 0.8$
$T_0 = 1600^\circ$K
$\lambda = 0.4$

$u_0 = 3000$ m/sec
are known functions of $\eta$, since $\rho$, $T$, $Y_2$, and $Y_3$ are calculated by solving the "frozen mixing" problem.

The chosen independent variables are defined as:

$$f_2(\eta) = \frac{K_2 \rho}{m_2} \frac{Y_2}{m_3} \frac{Y_3}{m_5}$$

$\eta = \sqrt{2/\tau_0} \frac{y}{x}$.

Fig. 3 gives $f_1(\eta)$ for different values of hydrogen and air temperatures and different ratios of hydrogen to air velocities. In order to reduce the number of cases to be computed, it is important to realize that $f_1$ is fairly insensitive to these values.

Fig. 4 gives $f_2(\eta)$ under the same conditions. The cases we are interested in correspond to values of $f_2(\eta)$ much smaller than $f_1(\eta)Y_5$. Under such conditions, dissociation in the injector outer boundary layer triggers the fast reactions; the role played by the initiation reaction $0$ is purely marginal.

Now, according to §2.1, we may assume that the transition time between the radicals producing reactions and the action of the chain is so small a fraction of the ignition delay time, that each mole of atomic oxygen which enters in the mixing zone, coming from the injector outer boundary layer, must cause immediately the appearance of two moles of atomic hydrogen. This requirement gives the following integral continuity condition near the injec-
tor exit:

\[ t = \int_{0}^{\infty} \rho u \frac{y_6}{m_6} \, dy = 2 \int_{-\infty}^{\infty} \rho u \frac{y_5}{m_5} \, dy . \]  

(7)

If we assume that the boundary layer thickness is small compared to the ignition delay length, we may write, following \(^2\), the initial distribution of \( y_5 \) for the mixing region as a Dirac \( \delta \) function of \( y \), so that, close to \( \xi = 0 \), \( y_5 \) would be given by:

\[ y_5 = N m_5 \frac{e^{-\eta^2}}{\xi} , \]

where, according to (7), \( N \) may be written as:

\[ N = \frac{\left( k_2 \rho \frac{y_3}{m_3} \right)}{\beta (\rho u)^0 \sqrt{2 \pi e^0 u}} , \]  

(8)

\( \beta \) being a "non-uniformity factor" which takes into account the fact that \( \rho u \) is not constant across the initial region of the mixing zone.

The solution of Eq.(6) can be expressed as follows:

\[ y_5 = y_5^{(o)} + y_5^{(1)} \]  

(9)

where

\[ y_5^{(o)} = N m_5 \frac{e^{-\eta^2}}{\xi} X (\xi, \eta) , \]  

(10)

satisfies the homogeneous differential equation obtained equating to zero the left hand side of (6), with the boundary conditions \( X (0, \eta) = 1 \).
Similarly, the second term of the right hand side of (9)

\[ y(1) = \frac{e^{-\eta^2}}{\xi} Z(\xi, n), \quad (11) \]

is to be found as solution of the complete equation with homogeneous boundary conditions.

The yet unknown function \( X(\xi, n) \) appearing in (10) may be written as:

\[ X(\xi, n) = 1 + \sum_{n=1}^{\infty} \xi^n X_n(n), \quad (12) \]

\( X_n(n) \) being the finite solution of the Hermite equation

\[ \frac{d^2X_n}{dn^2} - 2n \frac{dX_n}{dn} - 2n X_n = -2 f_1(n) X_{n-1} \quad (13) \]

In a similar fashion, \( Z(\xi, n) \) may be obtained by using a power series expansion of \( \xi \)

\[ Z(\xi, n) = \sum_{n=2}^{\infty} \xi^n Z_n(n), \quad (14) \]

where the \( Z_n(n) \) satisfy the following ordinary differential equations

\[ \frac{d^2Z_n}{dn^2} - 2n \frac{dZ_n}{dn} - 4Z_n = 2f_2(n) e^{n^2} \quad (15) \]

\[ \frac{d^2Z_n}{dn^2} - 2n \frac{dZ_n}{dn} - 2n Z_n = -2f_1(n) Z_{n-1}; \quad n > 2 \quad (16) \]
FIG. 5 $X_n$ vs $n$  
$T_P = 1000^\circ K$  
$u_o = 3000$ m/sec.
FIG. 6 - $Z_n$ vs $n$. $T_p = 1000^\circ$K. $u_o = 3000$ m/sec.

$T_o = 1300^\circ$K

$\lambda = 0.4$
$T_o = 1600^\circ K$
$
\lambda^o = 0.8$

FIG. 7 - $Z_n$ vs $n$. $T_F = 1000^\circ K$  $u_o = 3000$ m/sec.
The equation giving \( X_1(n) \) can be reduced to quadratures leading to:

\[
X_1(n) = \sqrt{\pi} e^{n^2} \left[ \text{erfc} \left( \int_{-\infty}^{n} f_1 dn \right) - \int_{-\infty}^{n} f_1 \text{erfc} dn \right] \left[ \frac{\text{erf} \left( \int_{-\infty}^{n} f_1 dn \right) + \frac{1}{2} \int_{-\infty}^{n} f_1 \text{erfc} dn \right]}{\sqrt{\pi} e^{n^2}} \right] (17)
\]

where

\[ \text{erfc} n = 1 - \text{erf} n \]

The remaining coefficients of the power series expansions (12) and (14) are not so easily calculated, since the general solutions of the corresponding homogeneous differential equations are Hermite series, so that they have been numerically computed by using an iterative procedure based on an expression similar to Eq.(17).*

Figs. 5 to 7 represent \( X(n) \) and \( Z(n) \) in two particular cases.

It is possible to improve the convergence of the power series expansion (12) by recasting \( X(\xi, n) \) as an exponential function

\[
X(\xi, n) = \exp \left[ \sum_{n=1}^{\infty} \xi^n X_n'(n) \right]
\]

where

\[
X_1'(n) = X_1(n)
\]

\[
X_2'(n) = X_2(n) - \frac{X_1(n)}{2}
\]

\[
X_3'(n) = X_3(n) - X_1(n) X_2(n) + \frac{X_3(n)}{3}
\]

* The computations were performed by F. Sanchis and A. Peña of IBM, S.A.E., using an IBM 360/40, and by J.M. Valero of INTA.
FIG. 8 - $\gamma(\phi/N)$ vs $\eta$ FOR DIFFERENT VALUES OF $\xi$

$T_0 = 1300^\circ$K, $\lambda = 0.4$

$T_F = 1000^\circ$K $u_o = 3000$ m/sec.
This series expansion has the advantage that the first term gives the exact behavior of $\chi(\xi,\eta)$ when $|\eta|$ is large, what suggest that, for finite values of $\eta$, this expression would be more accurate than the power series expansion in terms of $\chi_1(\eta)$. The extremely fast decrease of $\chi$ as $n$ increases corroborates this idea.

In a similar manner

$$Z(\xi,\eta) = \xi Z_2(\eta) \exp \left[ \sum_{n=1}^{\infty} \xi^n Z_n'(\eta) \right]$$

Fig.8 represents $\chi^0 (\xi,\eta)/N$ when $T_0 = 1300^{\circ}K$ and $\lambda = 0.4$, while Fig.9 shows the maximum value of this function versus $\xi$. The maximum values corresponding to $T_0 = 1600^{\circ}K$, $\lambda = 0.8$ are very similar to those represented in Fig.9. This fact is not surprising provided $f_1(\eta)$ is fairly insensitive to the conditions outside the mixing zone, as shown in §3.1. Fig.9 will be used hence-forth to calculate the ignition delay length.

The values of $\chi^1 (\xi,\eta)$ in both cases considered have been plotted in Figs. 10 and 11.

3.2 The Initial Concentration of Atomic Oxygen

In order to study the influence of dissociation in the injector outer boundary layer on the ignition delay length, let us begin estimating the amount of atomic oxygen introduced in the mixing layer from the air stream. It must be pointed out that, although the deceleration of the incoming air is limited as much as possible in order to avoid the air dissociation, some degree of dissociation in the injector boundary layer is in most cases unavoidable due to the high local temperature existing in
FIG. 9 - MAXIMUM VALUE OF $Y_5^{(o/N)}$ vs $\xi$

$T = 1000\degree K$ $u_o = 3000$ m/sec.

$T_0 = 1300\degree K$ $\lambda = 0.4$
FIG. 10 - $y_5^n$ vs $n$ FOR DIFFERENT VALUES OF $\xi$

$T_o = 1300^\circ K$  
$\lambda = 0.4$

$T = 1000^\circ K$  
$u_0 = 3000 \text{ m/sec.}$
FIG. 11 - $v_s^{(1)}$ vs $\eta$ FOR DIFFERENT VALUES OF $\xi$

$T_0 = 1600^\circ K$
$\lambda = 0.8$

$T_f = 1000^\circ K$
$u_0 = 3000$ m/sec.
that zone.

Fig. 12, plots values of \( N \) versus the maximum temperature in the injector outer boundary layer for a given pressure \( p \), outer velocity \( u_0 \) and injector length \( l \). These curves have been calculated by using the values of \( I \) obtained in \(^2\), following \(^6\); and Eq. (8) rewritten in the form:

\[
N = I \frac{2\sigma}{\beta \sqrt{\pi}} \frac{K_2 \left( \frac{Y_3}{m_3} \right)}{u_0^2 (1 + \lambda)}
\]

where \( \sigma = \sqrt{U/2\epsilon_\infty} \).

Two not very well defined factors appear in (8a): the jet spread parameter \( \sigma \) and the non-uniformity factor \( \beta \).

It has been deduced \(^7\), from the analysis of some experimental data, that the compressible jet spread parameter has an upper limit as the free stream Mach number approaches infinite. However no reliable information exists to be used when hydrogen mixes with air.

The computation of \( \beta \) will require additional numerical work out of the scope of this paper.

In calculating the values plotted in Fig. 12 it has been assumed \( \sigma/\beta = 50 \). It must be pointed out that \( N \) is rather insensitive to the particular value of \( \sigma/\beta \) chosen, since by doubling \( \sigma/\beta \), \( N \) increases in the same amount as by multiplying \( T_{max} \) by a factor of 1.02.

It may be seen from Fig. 12, that \( N \) strongly depends on the maximum temperature in the injector outer boundary layer and, consequently, on the maximum allowable temperature in the injector outer wall.
Concerning the influence of \( p, u \) and \( l \) on the values of \( N \); it is shown\(^2\) that \( N \sim (pl)^{3/2}/u_o^{1/2} \) so that \( N \sim (pl/u_o)^{3/2} \). 

\( T_0 \) influences \( N \) through \( T_{max} \) and \( k_2 \).

Finally, from Figs. 8 to 12 it is deduced that unless \( T_{max} \) is very low, dissociation in the injector outer boundary layer controls the ignition mechanism.

### 3.3 The Ignition Delay Zone Length

Once calculated \( N \), let us return to Eqs. (9), (10) and (11).

According to \$2\), we agree to define the end of the ignition delay zone as the value of \( \xi \) for which the reverse reaction 1 is of the same order as the forward reaction 2 at a local point \( n \).

Since under the validity of our approximation we have

\[
\frac{Y_5}{m_5} = \frac{Y_1}{n_1}
\]

throughout the ignition zone, we get the maximum value:

\[
\left( \frac{Y_5}{m_5} \right)_{max} = \frac{X_2}{K_1} \frac{Y_3}{m_3}
\]

where the left hand side is a known function of \( n \) as illustrated in Fig. 13 for the two typical cases considered throughout this paper.

Now, once \( N \) is known, it is possible to calculate the value of \( \xi \) corresponding to \( (Y_5/m_5)_{max} \), and the ignition delay time \( \tau \) which is given by

\[
\tau = \frac{\xi}{U} = \frac{\xi}{U} \left( K_2 \rho \frac{Y_3}{m_3} \right) \quad (22)
\]
FIG. 13 \( \frac{K_2}{K_{-1}} \frac{Y_3}{m_3} \) vs \( n \)

\[ T_0 = 1300^\circ K \quad \lambda = 0.4 \]
\[ T_0 = 1600^\circ K \quad \lambda = 0.8 \]

\( T_0 = 1000^\circ K \quad u_o = 3000 \text{ m/sec.} \)
The ignition delay time $\tau$ is plotted in Fig.14 versus the injector outer wall temperature $T_w$, in two typical cases. $T_w$ is related to $T_{\text{max}}$, under the assumption that air behaves as a "model fluid" ($\text{Pr}=1$, $\nu = \kappa\text{T}$), by the simple equation:

$$\frac{T_{\text{max}} - T_o}{T_w - T_o} = \frac{1}{4} \left[ \frac{1}{\alpha} + 1 \right]$$

where

$$\alpha = \frac{u_o^{2/2}}{c_p(T_w - T_o)}$$

The following remarks concerning Fig.14 should be emphasized:

a) The weak dependence of the ignition delay time $\tau$ on the injector outer wall temperature $T_w$ for large values of the outer temperature $T_o$ is noted. This is related to the well known fact that ignition delay times measured by different research groups, on premixed systems, correlate better when the temperature is large.

b) $\tau$ is nearly proportional to $p^{-1}$, according to Eq.(22), since the dependence of $N$ on the pressure $p$ is purely marginal.

c) Similarly, $\tau$ is almost independent of the injector length $l$ and the outer velocity $u_o$.

Points labelled A, A', B and B' in Fig.14 have been plotted in Fig.15, in order to make a comparison with the ignition delay data for premixed hydrogen-oxygen-diluent systems quoted by Nicholls et al.3.

The aim of Fig.15 is not to test the validity of the
Figure 14 - $T$ vs. injectors outer wall temperature $T_w$.

- $T = 10000 \text{ K}$
- $u_0 = 3000 \text{ m/sec.}$
- $T_0 = 16000 \text{ K}$
- $\lambda = 0.8$
FIG. 15 - $\tau$ vs $T_0$. $O_2$ CONCENTRATION FOR A, B, A', AND B' COMPUTED AT $n = 1.6$
present theory, which includes lateral diffusion effects, against data obtained under premixed conditions, but to point out that, provided the initial dissociation level is high enough, low delay times result in diffusional configurations.

IV. AERODYNAMIC FIELD NEAR THE INJECTOR EXIT

4.1 Flow Configuration at Low Injection Rates

The fact that the static pressure along the jet axis is not constant when hydrogen is injected parallel to a high speed stream of co-flowing air has been pointed out by Zakkay and Krause.

Fig.16a, taken from, shows static pressure measurements along the jet axis when there is no injection and when the momentum of the fuel injected \( \rho_F u_F \) is small compared with the outer flow momentum \( \rho_O u_O \).

When there is no injection, the pressure distribution is that corresponding to a near wake behind an obstacle at supersonic speeds. Close to the base the pressure decreases due to the expansion fan formed when the streamlines are bent inwards, and it again increases, due to the formation of shock waves, when the streamlines approach the jet axis (Fig.16b). The adverse pressure gradients produce recirculation in the wake due to the fact that the fluid particles inside the mixing zone do not have enough total pressure and are obliged to bend backwards. Later on, these particles are entrained to the mixing zone and replaced by new ones.

Fig.16a shows that when \( \rho_F u_F / \rho_O u_O \) is small (which seems to be the case when hydrogen is used as fuel) the pressure distribution and the flow configuration outside the wake remain
FIG. 16b - RECIRCULATION ZONE SCHEMATIC
NO INJECTION
FIG. 16c - RECIRCULATION ZONE SCHEMATIC
LOW INJECTION RATE
practically unchanged. Some experimental evidence seems to indicate that the near wake configuration is similar to what is shown in Fig.16c. When the total pressure of the fluid injected is small, the fuel cannot overcome the adverse pressure gradient along the axis, so that it bends outwards undergoing a process of mixing and recirculation. If the total pressure of the injected fuel goes up, the size of the recirculation bubble decreases while the flow field outside the wake is not so greatly affected.

It should be pointed out that according to experimental data presented in Fig.16a, a wake-like configuration appears even for fairly large fuel to air velocity ratios provided hydrogen is used as fuel. For example when $T_o = 1600^\circ K$, $T_F = 1000^\circ K$ and $\lambda = u_F/u_o = 1, \frac{\rho_F u_F}{\rho_o u_o}$ takes the value 0.09.

Needless to say that low values of the fuel to air velocity ratio favour the wake-like configuration, but significantly large injector areas should be used if a given amount of fuel is to be injected. Since the injector diameter is the characteristic length of the jet, the geometric scale of the flow pattern, and hence the combustor length, would increase.

On the other hand, large values of $\lambda$ should be avoided since the air entering in the mixing zone could be excessively cooled due to the low hydrogen temperature; moreover the maximum fuel temperature is limited by the structural materials.

It is concluded that in most cases of interest a wake-like configuration appears downstream of the injector exit, whose recirculating bubble improves the mixing and sends radicals backwards; these radicals, coming in contact with the hydrogen jet, trigger the fast reactions.

* Notice that these values are not those corresponding to the mixing zone, which is affected by the outer expansion and by the inner recirculation.
Some analytical work has been done by Carrière on two-dimensional wakes with small injection rates.

Essentially the said analysis gives the position of the dividing stream-lines at separation and reattachment as a function of the mass and momentum injected in the wake. In order to write down the balance of mass and momentum in the wake, it is assumed that the fluid injected does not disturb the velocity and temperature profiles corresponding to the wake with no injection.

Although it is likely that the last assumption ought to be reconsidered when hydrogen is injected (due to its low temperature and high specific heat) it should be remarked that this analysis also predicts that the wake is extremely insensitive to the injection rates of concern.

Now let us give an idea on the injector diameters required to get near wake lengths of the same order that the ignition delay lengths computed in §3.3, Fig.14.

From the analysis of some experimental data on supersonic wakes without injection, it is deduced that the recirculation zone length measured along the dividing stream-line, is of the order of one to two base (or injector) diameters, or even larger for transitional wakes. Since the delay lengths calculated in Fig.14 range from 0.6 cms (Point A') to 3.2 cms (Point B), it is concluded that in most cases of interest the distance between separation and reattachment is comparable to the ignition delay length.
DISCUSSION

The less satisfactory aspects of the approach presented above are due to the poor knowledge of turbulent mixing processes, even in the simple case of a non-reacting constant pressure shear layer. Owing to incertitude in the mixing mechanism and in the values of chemical reaction rates under turbulent conditions, the distribution of atomic hydrogen across the mixing zone shown in Fig. 8 may be open to criticism. Moreover this distribution is expected to highly influence the effectiveness of recirculation to improve the ignition process, since atomic hydrogen recirculates provided a substantial amount of it is present within the domain bounded by the dividing streamlines, whose positions correspond to values of \( n \) close to 0.2.

Second point concerns the extreme complexity of the recirculating configuration. The key to the solution of this problem is the strong interaction between the viscous flow originating in the boundary layer and free shear layer, and the external inviscid flow. The following refinements, under the present state of the art, have not been included in the simple free shear layer model assumed in the paper: a) The similar velocity profiles are only valid far from the body shoulder or injector edge. In some cases the separated layer is far too short for a similar solution to be valid on any point\(^{13}\). b) The compression along the wake axis is a smooth process, rather than the sudden compression assumed earlier\(^ {14}\). c) It has been suggested that the separation point is placed on the rear face of the body or injector edge and not at the corner as usually assumed\(^ {15}\). It is expected, however, that the introduction of these refinements will merely complicate the analytical treatment of the problem.

In addition, the study of the size and shape of the recirculation zone under low injection rate conditions is an interesting problem not sufficiently well understood. Some work has
been devoted to clarify this point, which is worth of being investigated further.

From the chemical point of view there are two more topics which need further discussion. The first one deals with assumptions leading to the over-all chemical reaction considered in the paper. It has been assumed that reactions 1 and 3 are infinitely fast, which obviously is true provided the delay time is large enough.

The second one concerns the possible production of nitric oxide in the injector outer boundary layer and its entrance in the mixing zone. Some experimental evidence seems to indicate that NO in very small quantities accelerates the $\text{H}_2-\text{O}_2$ reaction, while in larger quantities it inhibits the said reaction.

**CONCLUSIONS**

This paper presents a study of the ignition delay in supersonic air-subsonic hydrogen configurations under conditions of turbulent two dimensional mixing, and for pressures and temperatures significant to supersonic combustion.

It is shown that dissociation in the injector outer boundary layer produces oxygen atoms that, once introduced in the mixing layer, trigger the fast reactions and decrease the ignition delay length. This effect of decreasing the ignition delay length depends chiefly on the injector outer wall temperature and it is more remarkable the lower it is the free stream boundary temperature.

Under conditions of high production of radicals at the injector outer boundary layer, the ignition delay lengths are not too
unfavourably compared to those experimentally measured in premixed systems.

In addition, it is shown that these ignition delay lengths are of the same order of magnitude than the length of the recirculation zone which, in most cases, appears downstream of the injector exit.

POSSIBLE RELATED EFFORTS

Some related problems which merit further consideration are:

a) Effect of more elaborate treatments of the mixing process on the distribution of principal species and radicals. In particular, a model incorporating Townsend's description of fully developed free turbulent shear flows\(^{18}\) should be considered.

b) Feasibility of the production of nitric oxide in the injector outer boundary layer, and its effectiveness to accelerate or inhibit the \(\text{H}_2-\text{O}_2\) reaction.

c) Internal pattern of the recirculating wake configuration at low injection rates.

d) Internal structure of hydrogen-air diffusion flame not so far from chemical equilibrium as in the case considered in the paper.


York 1964) pp. 3-29.


