Ignition Analysis in Supersonic Turbulent Mixing Layer

A. M. Tahsini

Abstract—Numerical study of two dimensional supersonic hydrogen-air mixing layer is performed to investigate the effect of turbulence and chemical additive on ignition distance. Chemical reaction is treated using detail kinetics. Advection upstream splitting method is used to calculate the fluxes and one equation turbulence model is chosen here to simulate the considered problem. Hydrogen peroxide is used as an additive and the results show that inflow turbulence and chemical additive may drastically decrease the ignition delay in supersonic combustion.

Keywords—Ignition, Mixing layer, Numerical simulation, Supersonic combustion, Turbulence

I. INTRODUCTION

THE interests in the development of propulsion system for high speed vehicles as scramjets have led to extensive studies of supersonic combustion phenomena up to now. However, these studies confront many unresolved problems and much research remains to be done. One of the principal difficulties encountered has arisen from the flow residence times being of the same order of magnitude as the ignition delay time within the combustion chamber. Rapid ignition process as well as fast and complete combustion is significant to decrease combustor length and weight in this situation. On a physical viewpoint, ignition within a supersonic flow give rise to problems related to the coupling between chemical kinetics and compressible, high temperature, turbulence fluid dynamics. On the other hand, the flow dynamics in an actual combustor is rather intricate due to various flow structures and shock wave interactions arise from complex geometry. So the reacting mixing layer established between two parallel fuel-air streams was quite attractive for fundamental studies have been done, as described below.

Ju and Niioka [1] have made analytical study on ignition of a laminar, two-dimensional, supersonic mixing layer of parallel streams of unpremixed oxidant and fuel, using a three-step reaction kinetics to predict the ignition distance and the effects of free shear, Mach number, and reaction rates on the ignition distance. They have also numerically predicted the ignition distance for hydrogen-air and methane-air laminar mixing layer using reduced kinetic mechanism [2, 3]. Da Silva et Al. [4] have numerically investigated the effect of initial temperature and velocity gradients on ignition distance in supersonic laminar hydrogen-air mixing layer and found that the flame always starts from the airside and the triple flame

structure is not present in cases studied. Im et Al. [5] have asymptotically analyzed the thermal ignition behavior in laminar supersonic mixing layer using one-step overall reaction and reported that the ignition distance, for the case where the speed of the air stream is greater than that of the hydrogen, first increases as the Mach number increases. But it decreases with further increase in Mach number by virtue of the increase in temperature in the mixing layer because of friction generated heat. They also have repeated this study using reduced reaction mechanism [6]. Nishioka and Law [7] have numerically studied the temperature effect on ignition in supersonic laminar hydrogen-air mixing layer using detail chemistry and found that there is a lower limit of the air stream temperature below which ignition in a scramjet combustor is not possible and at higher temperatures, radical proliferation rather than thermal runaway cause ignition. Fang et Al. [8] have numerically investigated the effect of initial pressure on ignition distance in supersonic laminar mixing layer in the presence of a pressure gradient. Tien and stalker [9] have computationally studied the effect of the initial conditions on the ignition distance in supersonic laminar hydrogen-air mixing layer using detail chemical kinetics and showed that the initial oxygen atom concentration has serious effect on ignition delay. There are few researches reporting such studies in the presence of turbulent phenomena. Chakraborty et Al. [10] have investigated the supersonic turbulent reacting mixing layer using various empirical DNS data. Zambon et Al. [11] have numerically predicted the ignition distance in supersonic turbulent mixing layer using automatic reduction procedure chemical kinetics, for various splitter lip thicknesses. As is clear, ignition distance estimation is one of the most important purposes in scramjet study and design, and it is favorite to reduce it. Zabaikin et Al. [12] have experimentally investigated the effect of hydrogen peroxide addition on ignition and combustion in supersonic hydrogen-air flow and found that it becomes possible to decrease abruptly the ignition delay, improve the flame stability, and increase the combustion efficiency by using small amounts of chemically active additives. In the present study, the supersonic turbulent hydrogen-air mixing layer is analyzed numerically using detail chemical kinetics. The effect of various parameters such as flow turbulence level, the presence of water vapor in flow and hydrogen peroxide addition on ignition location are predicted and discussed.

II. GOVERNING EQUATIONS AND NUMERICAL METHOD

According to the considered problem (supersonic combustion in a mixing layer), the two dimensional Reynolds

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averaged compressible Navier-Stokes equations governing the continuum flow representing the conservation of mass, momentum, energy, and species are used. The conservation equations are written in the following form [13].

$$\frac{\partial U}{\partial t} + \frac{\partial (F + F_v)}{\partial x} + \frac{\partial (G + G_v)}{\partial y} = ST \quad (1)$$

$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho e \\ \rho m_j \end{bmatrix} \quad F = \begin{bmatrix} \rho u \\ \rho uu + p \\ \rho uv \\ \rho uh \\ \rho um_j \end{bmatrix}$$

$$G = \begin{bmatrix} \rho v \\ \rho vu \\ \rho vv + p \\ \rho vh \\ \rho vm_j \end{bmatrix} \quad F_v = \begin{bmatrix} 0 \\ -\tau_{xx} \\ -\tau_{xy} \\ q_x - u\tau_{xx} - v\tau_{xy} \\ \rho D_{eff} m_{j_x} \end{bmatrix} \quad (2)$$

$$G_v = \begin{bmatrix} 0 \\ -\tau_{yx} \\ -\tau_{yy} \\ q_y - u\tau_{yx} - v\tau_{yy} \\ \rho D_{eff} m_{j_y} \end{bmatrix} \quad ST = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \dot{\omega}_j \end{bmatrix}$$

$$\tau_{xx} = \mu_{eff}\left(2\frac{\partial u}{\partial x} - \frac{2}{3}\nabla.V\right)$$

$$\tau_{xy} = \mu_{eff}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) \quad (3)$$

$$\tau_{yy} = \mu_{eff}\left(2\frac{\partial v}{\partial y} - \frac{2}{3}\nabla.V\right)$$

$$\mu_{eff} = \mu + \mu_t$$
$$e = c_v T + (uu + vv)/2 + \sum m_j \Delta h_{f,j}^o$$
$$q = -k_{eff}\nabla T - \rho D_{eff}\sum h_i \nabla m_i \quad (4)$$
$$h_i = \Delta h_{f,i}^o + \int c_{p_i} dT$$

The turbulence model used to close the system of equations is the Spalart-Allmaras model [14]. This is a one-equation model assembled using empiricism and arguments of dimensional analysis, Galilean invariance, and selective dependence on the molecular viscosity. The eddy viscosity is determined through a partial differential equation as follows.

$$\frac{D(\tilde{v})}{Dt} = c_{b1}\tilde{S}\tilde{v} + \frac{1}{\sigma}\left[\nabla.((v+\tilde{v})\nabla\tilde{v}) + c_{b2}(\nabla\tilde{v})^2\right]$$
$$- c_{w1}f_w\left(\frac{\tilde{v}}{d}\right)^2 \quad (5)$$

This equation is solved for the variable $\tilde{v}$ and the eddy viscosity is calculated as $v_t = \tilde{v}f_{v1}$ where the function f_{v1} is a damping function used to treat the buffer layer and the viscous sublayer.

$$\tilde{S} = S + (\tilde{v}/\kappa^2 d^2)f_{v2}$$
$$f_{v2} = 1 - X/(1 + Xf_{v1})$$
$$f_{v1} = X^3/(X^3 + c_{v1}^3) \quad (6)$$
$$X = \tilde{v}/v$$

Here, d is the distance to the closest wall, S is the magnitude of vorticity, and $\tilde{S}$ is modified strain rate. The function f_w is given as

$$f_w = g\left(\frac{1 + c_{w3}^6}{g^6 + c_{w3}^6}\right)^{\frac{1}{6}} \quad (7)$$

Where

$$g = z + c_{w2}(z^6 - z)$$
$$z = \frac{\tilde{v}}{\tilde{S}\kappa^2 d^2} \quad (8)$$

The constants are: $c_{b1} = 0.1355$, $c_{b2} = 0.622$, $c_{v1} = 7.1$, $\sigma = 2/3$, $c_{w1} = 3.239$, $c_{w2} = 0.3$, $c_{w3} = 2$, $\kappa = 0.41$.

Equation (5) is solved coupled with flow governing equations.

The finite-rate reaction model (Table 1) which was given by Stahl and Warnatz is employed here as a full chemistry for hydrogen-air combustion [15]. There are nine chemical species within reaction mechanism so eight conservation equations for species should be considered beside one overall mass fraction equation. Therefore, there are thirteen coupled equations to be solved in flow field. Cell centered based finite volume method is used to discrete the governing equations. The time

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integration is accomplished by an explicit time stepping scheme [16]. Viscous terms are calculated using a central scheme and inviscid terms are treated using an AUSM+ method (Advection Upstream Splitting Method) to express the numerical flux at cell faces [17]. This method is one of the most recent developed ones which is faster than the famous Roe's scheme and has following features: Positivity preserving property, improvement in accuracy, simplicity, and easy generalization to other conservation laws. The present simulation program has been validated using variety of benchmark problems and used successfully to study the solid fuel ignition in turbulent flows [18-20].

TABLE I
CHEMISTRY MODEL

Mechanism				A (cm/mol/s)	Exp of T	E (kJ/mol)
O_2 +H		→ OH	+O	2.20E + 14	0.00	70.30
OH +O		→ O_2	+H	1.72E + 13	0.00	3.52
H_2 +O		→ OH	+H	5.06E + 04	2.67	26.30
OH +H		→ H_2	+O	2.22E + 04	2.67	18.29
H_2 +OH		→ H_2O	+H	1.00E + 08	1.60	13.80
H_2O +H		→ H_2	+OH	4.31E + 08	1.60	76.46
OH +OH		→ H_2O	+O	1.50E + 09	1.14	0.42
H_2O +O		→ OH	+OH	1.47E + 10	1.14	71.09
H +H +M*		→ H_2	+M*	1.80E + 18	-1.00	0.00
H_2 +M*		→ H	+H +M*	7.26E + 18	-1.00	436.82
H +OH +M*		→ H_2O	+M*	2.20E + 22	-2.00	0.00
H_2O +M*		→ H	+OH +M*	3.83E + 23	-2.00	499.48
O +O +M*		→ O_2	+M*	2.90E + 17	-1.00	0.00
O_2 +M*		→ O	+O +M*	6.55E + 18	-1.00	495.58
H +O_2 +M*		→ HO_2	+M*	2.30E + 18	-0.80	0.00
HO_2 +M*		→ H	+O2 +M*	3.19E + 18	-0.80	195.39
HO_2 +H		→ OH	+OH	1.50E + 14	0.00	4.20
H +OH		→ HO_2	+H	1.50E + 13	0.00	170.84
HO_2 +H		→ H_2	+O_2	2.50E + 13	0.00	2.90
H_2 +O_2		→ HO_2	+H	7.27E + 13	0.00	244.33
HO_2 +H		→ H_2O	+O	3.00E + 13	0.00	7.20
H_2O +O		→ HO_2	+H	2.95E + 13	0.00	244.51
HO_2 +O		→ OH	+O_2	1.80E + 13	0.00	-1.70
OH +O_2		→ HO_2	+O	2.30E + 13	0.00	231.71
HO_2 +OH		→ H_2O	+O_2	6.00E + 13	0.00	0.00
H_2O +O_2		→ HO_2	+OH	7.52E + 14	0.00	304.09
HO_2 +HO_2		→ H_2O_2	+O_2	2.50E + 11	0.00	-5.20
OH +OH +M*		→ H_2O_2	+M*	3.25E + 22	-2.00	0.00
H_2O_2 +M*		→ OH	+OH +M*	1.69E + 24	-2.00	202.29
H_2O_2 +H		→ H_2	+HO_2	1.70E + 12	0.00	15.70
H_2 +HO_2		→ H_2O_2	+H	1.32E + 12	0.00	83.59
H_2O_2 +H		→ H_2O	+OH	1.00E + 13	0.00	15.00
H_2O +OH		→ H_2O_2	+H	3.34E + 12	0.00	312.19
H_2O_2 +O		→ OH	+HO_2	2.80E + 13	0.00	26.80
OH +HO_2		→ H_2O_2	+O	9.51E + 12	0.00	86.68
H_2O_2 +OH		→ H_2O	+HO_2	5.40E + 12	0.00	4.20
H_2O +HO_2		→ H_2O_2	+OH	1.80E + 13	0.00	134.75

III. RESULTS AND DISCUSSION

At first, the focus is on problem has been examined by Ju and Niioka [2], the autoignition process within laminar mixing layer between a supersonic air stream and a hydrogen stream diluted by nitrogen neutral gas (Fig. 1).
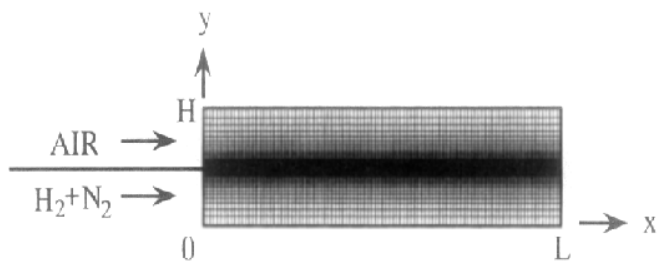

Fig. 1 Schematic configuration of problem [2]

At $T_{air} = T_{H2}=1200\ K$ and $M_{air}=1.84$, $M_{H2}=1.2$, the ignition distance was reported *9.6 cm* downstream of the splitter. The present study has exact agreement with Ref. 2. Temperature distribution along splitter is shown in Fig. 2 and temperature

contours show the flame position in flow field in Fig. 3. It emphasizes again the validity of present numerical procedure.
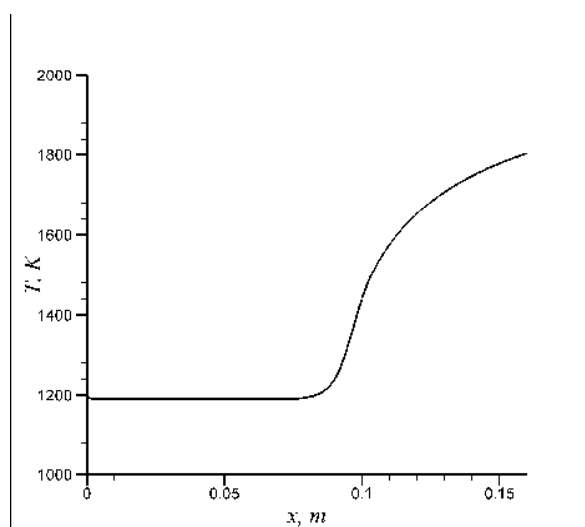

Fig. 2 Temperature along splitter.

Fig. 3 Flame position

As mentioned earlier, ignition location is an important subject in supersonic combustion propulsion systems and its reduction will help scaling down the scramjets. Some effective parameters on this subject are studied here.

A. Inflow turbulence

The problem under consideration has a turbulence transition distance longer than the specified geometry [21]. So the inside generated turbulence effect is not important here. The focus is on the inflow turbulence influence. To study this, the ignition simulation is re-examined using various inflow turbulence levels.
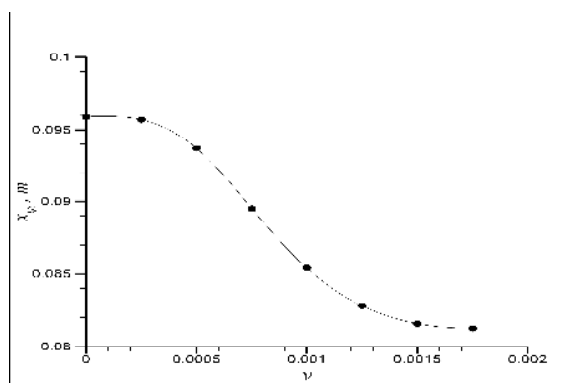

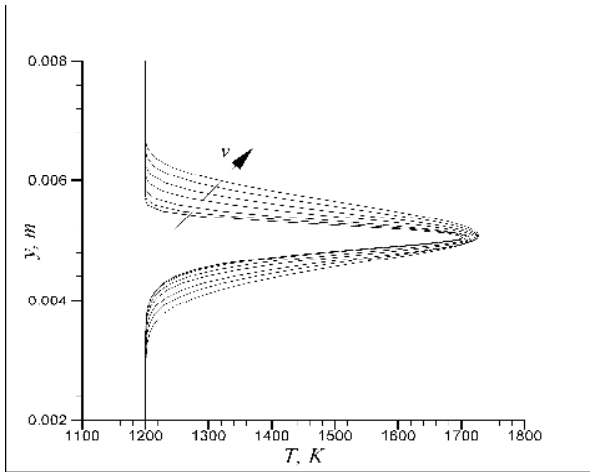Fig. 4 Ignition distance variation due to turbulence

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Fig. 5 Lateral distribution of temperature

The results show that increasing the turbulence level up to certain level (eddy viscosity of about *0.0015* for this situation), decreases the ignition distance about fifteen percent and amplify the flame thickness. But more than this level, it just increases the flame thickness and has no effect on ignition delay. Figure 4 displays the ignition location versus inflow turbulence. Figure 5 illustrates the flame thickness increment by the lateral distribution of temperature at 3 cm downstream the ignition location. Flame widening is appropriate to avoid combustion instabilities in propulsion systems achieved here by inflow turbulence.

B. Hydrogen peroxide additive

Using hydrogen peroxide as an additive has intense influence on ignition delay reduction. It is shown here by adding a little H_2O_2 to flow in different three ways: First by adding it to fuel flow instead of nitrogen, then adding it to fuel instead of hydrogen and finally adding it to air instead of nitrogen up to one percent. Ignition distance variation versus H_2O_2 mass fraction is presented in Fig. 6. The results show that it is not important to add the additive instead of which species, but the addition to air has more effect than fuel flow. Furthermore, although a little hydrogen peroxide addition decreases suddenly the ignition delay, increasing its mass fraction slowly continues this reduction.
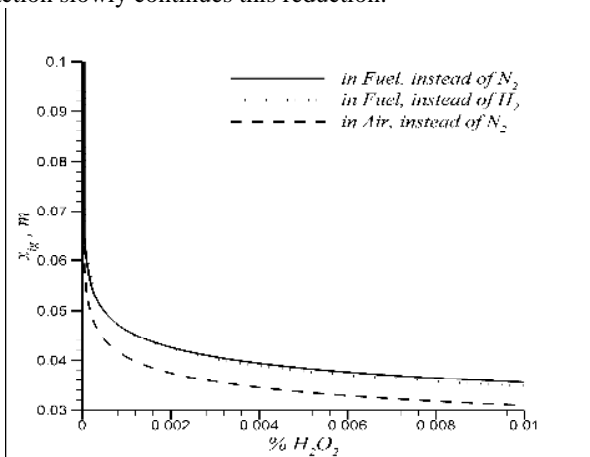

Fig. 6 Ignition distance variation due to H_2O_2 addition

C. Inflow water vapor

Presence of the water vapor within inflow air may alter the ignition process in propulsion with air intake like scramjets. Adding a little vapor in air increases the ignition distance as expected primarily which is not favorable (Fig. 7). Examining more vapor addition indicates strange result contrary to expectation. Increasing water vapor mass fraction a little more than about two percents in this situation suddenly decreases the ignition distance and after that the initial behavior recurs and ignition distance increases (Fig. 8). It is interesting that for about *2.5%* vapor, the ignition distance is smaller than the elementary dry air condition.
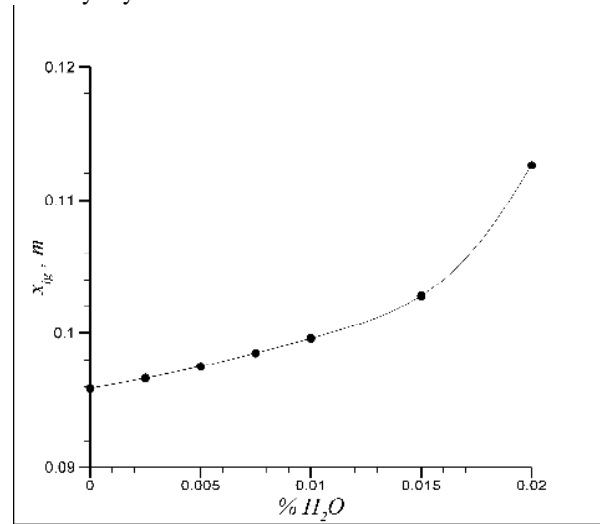

Fig. 7 Ignition distance versus vapor mass fraction in air flow
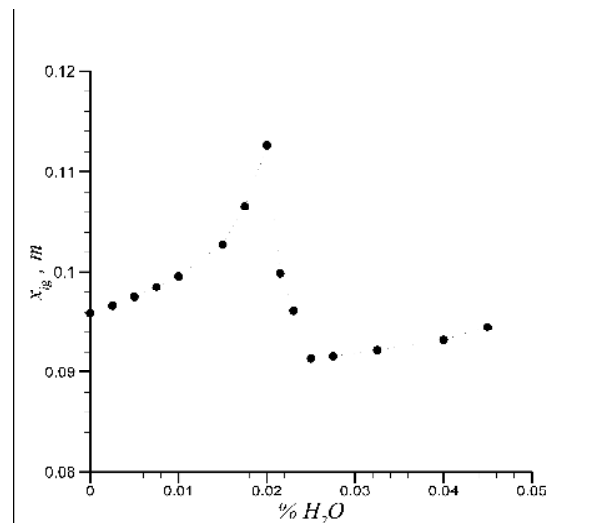

Fig. 8 Ignition distance versus much more vapor mass fraction in air

flow

Water vapor value cannot be controlled at air inlet simply but inflow turbulence and using additive may apply to decrease the ignition delay in scramjets. For example, using an inlet eddy viscosity of *0.001* and adding *0.1%* hydrogen peroxide to air decreases the ignition distance from initial *9.6 cm* to *3.7 cm* which is significant reduction. Figure 9 illustrates this by flame position in flow field.

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Fig. 9 flame position, *a*: base flow, *b*: turbulent flow with chemical additive

IV. CONCLUSION

In the present study, the ignition of hydrogen-air supersonic mixing layer is numerically analyzed using detail chemistry. Attention is paid to the ignition distance estimation and reduction by inflow turbulence level and H_2O_2 addition. It is shown that the increasing turbulence level decreases the ignition distance and widens the flame up to certain level, but more than it just increases the flame thickness which is favorable according to combustion stability. Also adding H_2O_2 to air or fuel flow decreases the ignition delay significantly and adding it to air is much better. Water vapor presence in air inlet has strange effect on ignition; its effect is not monotonic and has a discontinuous behavior. At first, vapor increment increases the ignition distance but in a certain value, there is sudden reduction in ignition distance and after that the initial behavior recurs. The results show that increasing the inlet turbulence level and using a little hydrogen peroxide may decreases the ignition distance for about one third of initial value.

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