

The application of turbulent kinetic theory to a reacting flow of turbulent plane jet

Shu-Hao Chuang

Department of Mechanical Engineering, National Chung-Hsing University, Taiwan, Republic of China

Zuu-Chang Hong

Department of Mechanical Engineering, National Central University, Taiwan, Republic of China, and

Jhy-Horng Wang

Department of Power Mechanical Engineering, National Tsing-Hua University, Taiwan, Republic of China

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Nomenclature

a	= radius of the round jet	\bar{U}_j	= velocity of the jets at the nozzle exit
C	= concentration mass fraction	\bar{U}_∞	= surroundings velocity
C_p	= specific heat at constant pressure	\bar{U}_M	= mixed center velocity
D	= diameter of the round jet or width of the jet	\bar{U}_0	= relative velocity ($\bar{U}_M - \bar{U}_\infty$)
E	= turbulent energy ($= u'^2 + v'^2 + w'^2$)	u, v, w	= instantaneous velocity in the x , y and z directions respectively
ΔE	= activation energy	u', v', w'	= fluctuation velocity in the x , y and z directions respectively
F	= probability density function of scalar $\alpha(t, x, y)$	$\bar{U}, \bar{V}, \bar{W}$	= average velocity in the x , y and z directions respectively
f	= pdf of the fluid element	x	= co-ordinate along the jets axis
f_0	= source condition pdf of the fluid element	y	= co-ordinate normal to the jets axis
$f(u), f(v), f(w)$	= pdf of the velocity in the x , y and z directions respectively	β_1	= characteristic relaxation rate of the energy-containing eddies
Δh_0	= heat of evolution of the chemical reaction	β^v	= characteristic relaxation rate of the microscale
K_f	= $K_f \exp(-\Delta E/RT)$ (specific reaction rate)	η	= $y/(x+2D)$
M	= molecular weight	Ω	= chemical reaction term
m	= dimensionless concentration of fuel	<i>Subscripts and superscripts</i>	
n	= dimensionless concentration of oxygen	- or <>	= average value
R	= gas constant or velocity ratio (\bar{U}_∞/\bar{U})	\rightarrow	= vector
$RF_{m,v}$	= pdf of the oxygen in v -direction velocity space ($= (30/142) F_{m,v}$)	∞	= freestream condition
$RF_{n,v}$	= pdf of the oxygen in v -direction velocity space ($= (112/142) F_{n,v}$)	0	= source condition
r	= co-ordinate along the radial direction	c	= inert gas
S_0	= source condition at $x = 0$	f	= fuel
\bar{T}	= average temperature	g	= oxygen
T'	= fluctuation temperature	j	= tensor
t	= time	p	= product
		t	= temperature

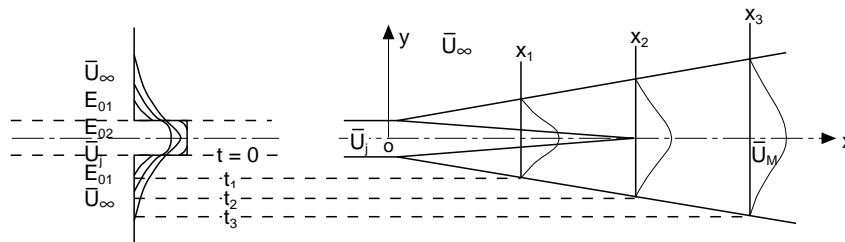
Introduction

Most of the approaches to turbulence modeling have been developed from the concept of gradient type-transport. But an alternate approach to turbulence modeling treats the turbulence statistically (Batchelor, 1960; Hinze, 1975). The classical statistical theories (Batchelor, 1960; Hinze, 1975; Taylor, 1935; Von Karman, 1937; Von Karman and Lin, 1949) of turbulence are mainly energy spectrum analyses, which deal with homogeneous and isotropic turbulence and are less attractive to engineers (Taylor, 1935; Von Karman, 1937; Von Karman and Lin, 1949). Since 1967 there have been some turbulent kinetic theories proposed, such as those of Lundgren (1969; 1975), Fox (1971), Yen (1972) and Haworth and Pope (1986). These theories were limited to the study of the flow field without chemical reaction. A more general kinetic theory of turbulence for chemically reacting flows was developed by Chung (1970; 1972; 1973).

Past solutions to Chung's kinetic equation have been considered for simple one-dimensional geometries and employed the approximated bimodal method of Lin and Lees (1961). In 1975 Chung's kinetic equation (Chung, 1967) was solved by Hong (1975) by a Green's function method. In the Green's function method, the Green's function of Chung's kinetic equation was first constructed and was employed to integrate over the source conditions according to the boundary conditions of the given physical problem to obtain the pdf (probability density function). A numerical solution of Chung's kinetic equation for a free shear layer was presented by Bywater (1981) in which the pdf considered was reduced to one component since the joint pdf of different components of fluctuations was not obtained. In Bywater's work, the cross correlations or high order moments were not shown in his results. The same kinetic theory was employed by Hong and Chuang (1988) to solve the twin plane jets turbulent mixing by using the modified Green's function method. The cross correlations of the fluctuations were described via the revealed joint pdf, $f(u, v)$, in Hong and Chuang's (1988) work. The modified Green's function method was also employed for the present analysis. In this method, an instantaneous mixing phenomenon was actually solved to simulate the steady-state mixing problem of Figure 1. Details of the method were given in a previous paper (Hong and Chuang, 1988).

Many salient features of the present kinetic theory approach to chemically reacting flows have been revealed previously (Bywater, 1982; Chung, 1967; 1970; 1972; 1973; Hong, 1975; Hong and Chuang, 1988). The flame zone

Figure 1.
(a) instantaneous mean velocity profiles observed at fixed x ;
(b) mean velocity profiles observed when moving with the velocity \bar{U}_M



structure could be revealed by the present kinetic theory approach even under the assumption of infinite fast chemical reaction rate. The gradient-type closure technique of the eddy viscosity concept for the same problem of a diffusion flame usually resulted in a flame sheet solution. But the experimental evidence showed that turbulent diffusion flame at very fast chemical reaction rate should be a flame zone instead of a flame sheet (Hawthorne *et al.*, 1949). Toor (1962) used the statistical approach and obtained a flame zone solution. In his analysis, a prescribed Gaussian distribution of the chemical species in the turbulent field was employed. Another statistical model developed by Lin and O'Brien (1974) and Bush and Fendell (1975) differed only by a different assumption of the prescribed pdf for species distribution in the turbulent reacting field. In the present analysis, we calculate the results for the reacting flow of a turbulent plane jet via Chung's (1967) kinetic theory approach. Once the pdf is obtained and a combustion model is assumed, one can proceed to calculate the properties of turbulent plane jet with chemical reaction; the species pdf distributions, species mass fraction distributions, temperature distributions, turbulent heat transfer, species mass transfer and flame structure are given in the present analysis.

Theoretical model

The starting point of the present analysis was the kinetic equations developed by Chung (1967) previously, which were given as:

$$\frac{\partial F_i}{\partial t} + u_j \frac{\partial F_i}{\partial x_j} = \beta \frac{\partial}{\partial u_j} (u_j - \langle u_j \rangle) F_i + \beta_1 \frac{E}{3} \frac{\partial^2 F_i}{\partial u_j \partial u_j} + \Omega \cdot \mathbf{f} \quad (1)$$

where

$$\beta = \beta_1 + \beta^v, F = c \cdot f, F = f \cdot c_1, \Sigma F_i = f \cdot \Sigma c_1 = f$$

Description of the flowfield of engineering interest is based on the probability density function $f(t, \bar{x}, \bar{u})$ in the present analysis. If the fluid element has a concentration of a scalar quantity of $c(t, \bar{x}, \bar{u})$, then the pdf of this scalar $c(t, \bar{x}, \bar{u})$, $F(t, \bar{x}, \bar{u})$, is:

$$\mathbf{F}(t, \bar{x}, \bar{u}) = \mathbf{c}(t, \bar{x}, \bar{u}) \cdot \mathbf{f}(t, \bar{x}, \bar{u})$$

For the present problem, Figure 2 shows the flowfield geometry of a turbulent plane jet. It consists of a jet stream which carries the fuel, while the surrounding environment carries the oxidizer and diluent (or air). The chemical reaction is according to the following one-step and one-direction combustion model:



where f , g and p represent the number of moles of each species. The instantaneous production rate of combustion products is given by:

$$\Omega_p = K \cdot \exp(-\Delta E / R \cdot T) \cdot C_r^f \cdot C_s^g \quad (3)$$

where K is a constant, and ΔE , R , T , Ω_p , C_r , C_s represent the activation energy, gas constant, absolute temperature, chemical production rate, mean mass fraction of fuel and oxidant. The instantaneous production rates of fuel Ω_r , oxidant Ω_s , and energy Ω_p due to chemical reactions are related to Ω_p

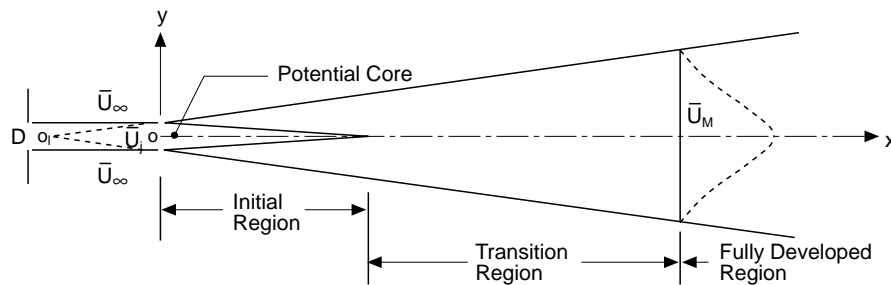


Figure 2.
The flowfield geometry
of turbulent plane jet

The full set of equations is represented by equation (1) with:

$$I = \begin{cases} r & \text{fuel} \\ s & \text{oxidant} \\ t & \text{temperature} \\ p & \text{product} \\ c & \text{inert} \end{cases}$$

The reaction terms can be eliminated in all except the equation for t with the transformation

$$\begin{aligned} F_m &= (PM_p / f M_r) F_r, & F_n &= (PM_p / g M_s) F_s \\ F_h &= (C_p / \Delta h_0) F_t, & F_\alpha &= F_m + F_h, & F_\beta &= F_n + F_h \end{aligned} \quad (4)$$

where Δh_0 , C_p , and M are the heat of reaction, specific heat, and molecular weight respectively. The result is the following equations for F , F , F_{β} :

$$\frac{\partial F_\alpha}{\partial t} + u_j \frac{\partial F_\alpha}{\partial x_j} = \beta \frac{\partial}{\partial u_j} [F_\alpha \cdot (u_j - \langle u_j \rangle)] + \beta_1 \frac{E}{3} \frac{\partial^2 F_\alpha}{\partial u_j \partial u_j} \quad (5)$$

$$\frac{\partial F_\beta}{\partial t} + u_j \frac{\partial F_\beta}{\partial x_j} = \beta \frac{\partial}{\partial u_j} [F_\beta \cdot (u_j - \langle u_j \rangle)] + \beta_1 \frac{E}{3} \frac{\partial^2 F_\beta}{\partial u_j \partial u_j} \quad (6)$$

$$\frac{\partial F_h}{\partial t} + u_j \frac{\partial F_h}{\partial x_j} = \beta \frac{\partial}{\partial u_j} [F_h \cdot (u_j - \langle u_j \rangle)] + \beta_1 \frac{E}{3} \frac{\partial^2 F_h}{\partial u_j \partial u_j} \quad (7)$$

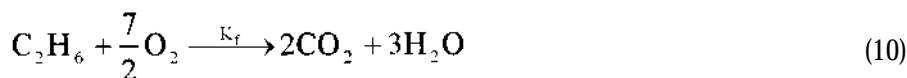
Equations (1) (with $1 = c$) and (5)-(7) as well as auxiliary relationships (3)-(4) govern the combustion of reactants in the plane turbulent jet. $(F_m)_i$ and $(F_n)_i$ are further defined to represent the values of F_m and F_n respectively, without chemical reaction. From equations (5) and (6), then:

$$(F_m)_i - (F_n)_i = F_m - F_n \quad (8)$$

If the chemical reaction rate is infinite, namely, $K_0 \rightarrow \infty$ (or $K_f \rightarrow \infty$), application of this limit to equation (2) has been shown to lead to the following result:

$$F_m \cdot F_n = 0 \quad (9)$$

Under the present restriction of infinite chemical reaction rates, the physical meaning of equation (9) is that the combustion can proceed when the fuel and oxidant appear simultaneously in the velocity cell. Therefore, the ability of the reactants to react depends upon their history in the turbulence field. In order to use the results of momentum without chemical reaction, one can choose the density of fuel, e.g. C_2H_6 , almost the same as that of the air. The reaction equation of C_2H_6 is:



According to the above mentioned physical problem, the source conditions of the reactants for mass fraction can be written as:

$$C_{2O} = C_{rO} = 1.0 \quad |y| \leq \frac{h}{2} \quad ; \quad X \leq 0 \quad (11)$$

$$C_{1O} = \begin{cases} C_{SO} = 0.22 \\ C_{CO} = 0.78 \end{cases} \quad |y| \geq \frac{h}{2} \quad ; \quad X \leq 0 \quad (12)$$

From equations (4) and (10):

$$m = \frac{142}{30} C_r \quad (13)$$

$$n = \frac{142}{112} C_s$$

Therefore, the source conditions m_0 and n_0 of the m and n become:

$$\left\{ \begin{array}{l} m_0 = 1.0 \times \frac{142}{30} \quad |y| \leq \frac{h}{2} \quad ; \quad X \leq 0 \end{array} \right. \quad (14)$$

$$\left\{ \begin{array}{l} n_0 = 0.22 \times \frac{142}{112} \quad |y| \geq \frac{h}{2} \quad ; \quad X \leq 0 \end{array} \right. \quad (15)$$

The major mixing direction of the fuel and oxidant for the turbulent plane jet is in y-direction, so equation (9) can be simplified as follow:

$$\mathbf{F}_{m,v} \cdot \mathbf{F}_{n,v} = 0 \quad (16)$$

where

$$\begin{cases} \mathbf{F}_{m,v} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathbf{F}_m(\bar{\mathbf{u}}) \, d\mathbf{u} \, d\mathbf{w} \\ \mathbf{F}_{n,v} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathbf{F}_n(\bar{\mathbf{u}}) \, d\mathbf{u} \, d\mathbf{w} \end{cases} \quad (17)$$

Equation (16) represents the pdf in velocity space which was simplified to the v-direction only. That is, the reaction process can occur only when the fuel and oxidant coexist in v-velocity space. The v-direction velocity space was further divided into v_m and v_n where v_m and v_n represent the velocity space of fuel and oxygen, respectively.

$$\begin{cases} (\mathbf{F}_{m,v})_i \geq (\mathbf{F}_{n,v})_i & \text{when } \mathbf{v} = \mathbf{v}_m \\ (\mathbf{F}_{m,v})_i \leq (\mathbf{F}_{n,v})_i & \text{when } \mathbf{v} = \mathbf{v}_n \end{cases} \quad (18)$$

where

$$\begin{cases} (\mathbf{F}_{m,v})_i = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (\mathbf{F}_m)_i \, d\mathbf{u} \, d\mathbf{w} \\ (\mathbf{F}_{n,v})_i = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (\mathbf{F}_n)_i \, d\mathbf{u} \, d\mathbf{w} \end{cases} \quad (19)$$

Therefore, equations (8) and (16) can be replaced by:

$$\begin{cases} \mathbf{F}_{m,v} = (\mathbf{F}_{m,v})_i - (\mathbf{F}_{n,v})_i & \text{when } \mathbf{v} = \mathbf{v}_m \\ \mathbf{F}_{n,v} = 0 \end{cases} \quad (20)$$

$$\begin{cases} \mathbf{F}_{n,v} = (\mathbf{F}_{n,v})_i - (\mathbf{F}_{m,v})_i & \text{when } \mathbf{v} = \mathbf{v}_n \\ \mathbf{F}_{m,v} = 0 \end{cases} \quad (21)$$

Equations (20) and (21) are the final results for the reaction process in the present model, with source conditions given by equations (14) and (15). The application of equations (20) and (21) in connection with the solutions for $F_{\alpha,v}$ and $F_{\beta,v}$ has, as a result, to obtain the solutions for $F_{m,v}$ and $F_{n,v}$.

Results and discussion

In order to make comparisons with available experimental data, two velocity ratios $R = 0$ and $R = 0.16$ are chosen in the present analysis. In the following paragraphs the calculated results of pdf distributions of chemical species, turbulent transport of chemical species, temperature distribution, turbulent heat transfer, and flame structure are discussed in detail. The mean velocity profile in the fully-developed region is compared with Wygnanski's (Gutmark and Wygnanski, 1976) experimental data and is found in reasonably good agreement (Chuang *et al.*, 1991). The turbulent energy distributions with velocity ratios $R = 0$ and $R = 0.16$ are compared with Wygnanski's (Gutmark and Wygnanski, 1976) and Bradbury's (Bradbury, 1965) experimental data respectively, and found in good agreement (Chuang *et al.*, 1991).

pdf distribution of chemical species

As mentioned above, equation (9) prohibits the coexistence of fuel and oxidant in the same probability density cell in vertical velocity space. According to this model, some of the probability distribution functions of fuel (C_2H_6), oxygen and product ($CO_2 + H_2O$) in v' -velocity space are shown in Figures 3-5. The species

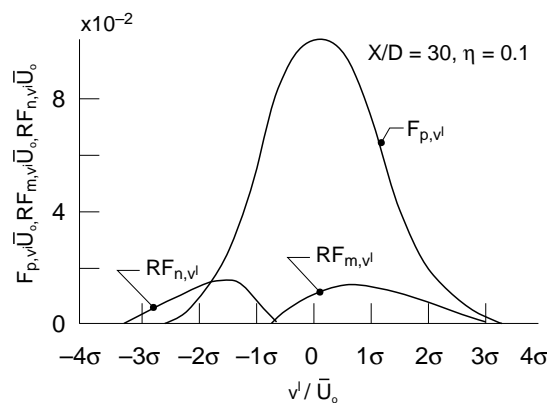


Figure 3.
Species pdf in v' -velocity
space ($R = \bar{U}_\infty / \bar{U}_0$,
 $X/D = 30$, $\eta = y / (X$
 $+ 2D) = 0.1$)

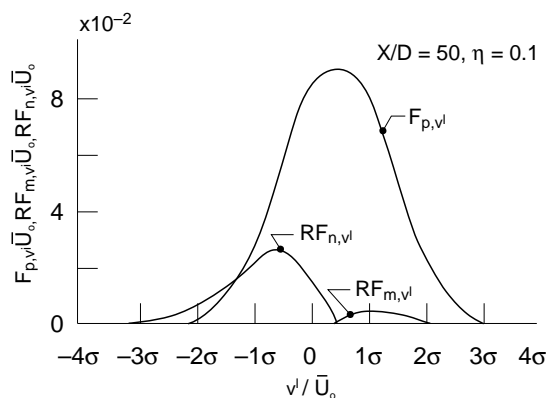
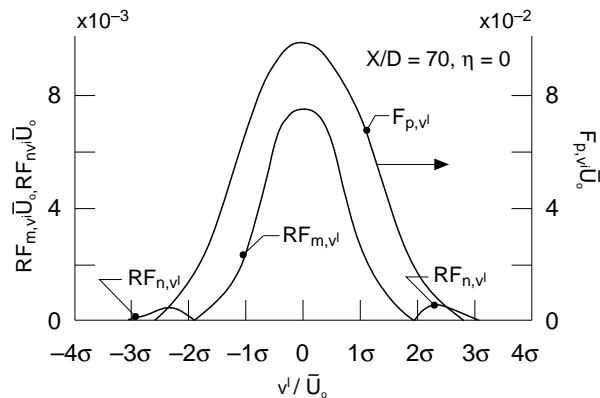


Figure 4.
Species pdf in v' -velocity
space ($R = 0$, $X/D = 50$,
 $\eta = 0.1$)

Figure 5.
Species pdf in v' -velocity
space ($R = 0, X/D = 70,$
 $\eta = 0$)



pdf in v' -velocity space at $X/D = 30, \eta = 0.1$ and $X/D = 50, \eta = 0.1$ are shown in Figures 3-4. In Figures 3 and 4, it can be seen that the oxygen diffuses from the negative side to the positive side at $\eta = 0.1$ as one proceeds downstream. This means that the diffusive mixing of fuel and oxygen at $X/D = 30-50$ will increase the effect of combustion. In Figure 5, it can be found that the oxygen appears in both negative and positive sides. This means that at this point oxygen comes from both directions, i.e. the positive and negative y -direction.

Distributions of chemical species

Figures 6-8 show the mass fraction distributions of chemical species at different cross sections. At $X/D = 10$, the mass fraction of oxygen diffuses only to $\eta = 0.11$, as shown in Figure 6, so the maximum products appear at $\eta = 0.11$. Along the downstream at $X/D = 30$, the oxygen has diffused to $\eta = 0.9$, as shown in Figure 7. The reacting zone is toward the axial direction when the flow is along with the downstream, as shown in Figures 6 and 7. At $X/D = 70$, the fuel is almost reacting with the oxygen, as shown in Figure 8. Because of the limited experimental data for turbulent plane jet combustion, only trends and general characteristics of the calculated results will be compared with Kent's (Kent and

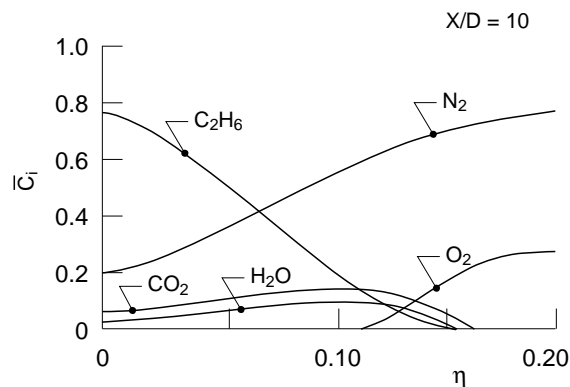


Figure 6.
Mass fraction
distributions of species
($R = 0, X/D = 10$)

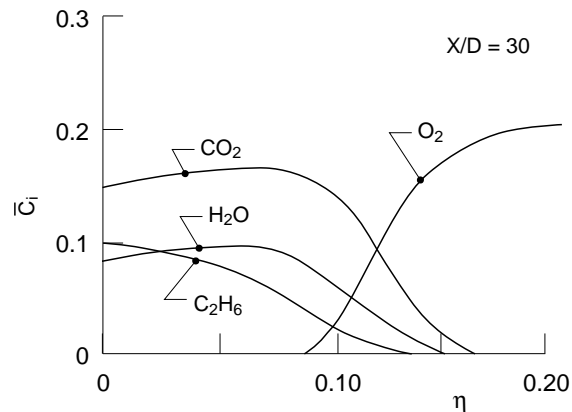


Figure 7.
Mass fraction
distributions of species
($R = 0$, $X/D = 30$)

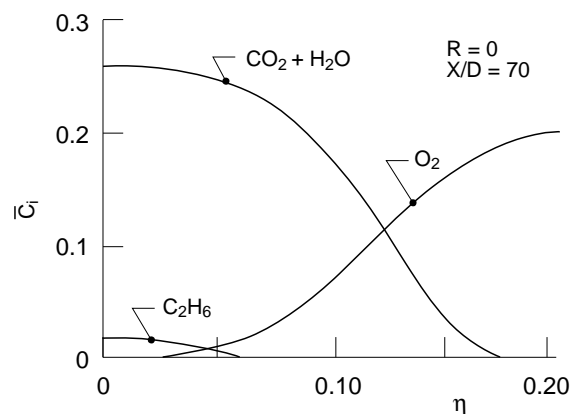


Figure 8.
Mass fraction
distributions of species
($R = 0$, $X/D = 70$)

Bilger, 1975) experimental data for turbulent round jet combustion. This comparison is shown in Figures 9-11. The fuel used in Kent's (Kent and Bilger, 1975) experiment is H_2 . It is found that the trends and general characteristics of the present calculations are in very good agreement with Kent's (Kent and Bilger, 1975) experimental data. Both Figures 9 and 10 show that the present results have a wider distribution than the experimental data, which is due to the fact that the plane jet has a wider mixing region than the round jet when the velocity ratios are the same (Hinze, 1975; Wygnanski and Fiedler, 1969). The fuel concentrations of the present results have a larger value than the experimental data because the fuel used in the present analysis is heavier than the fuel used in Kent's (Kent and Bilger, 1975) experiment, as shown in Figures 9 and 10. The O_2 concentration distributions along the centerline of the present results have a larger value than the experimental data owing to the difference of the fuel, as shown in Figure 11.

Figure 9.
Species' mass fraction
distributions compared
with Kent's data
($R = 0.2, X/D = 70$)

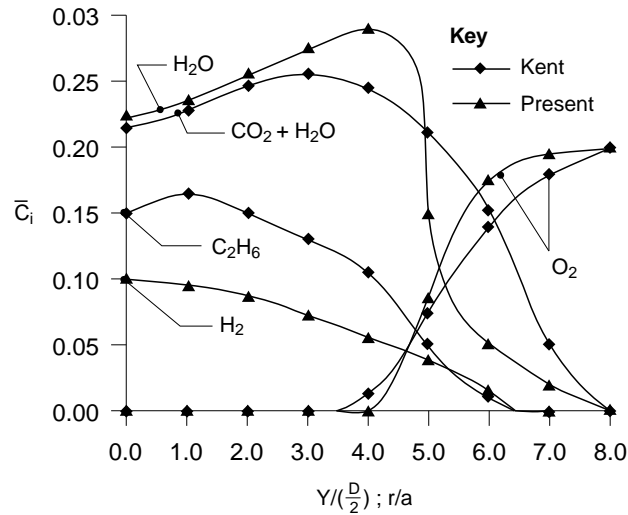
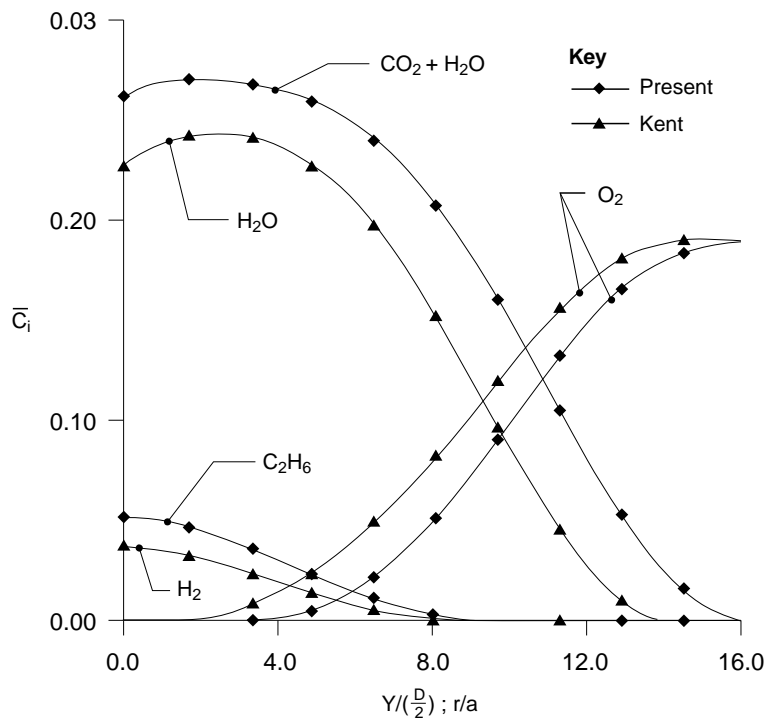


Figure 10.
Species' mass fraction
distributions compared
with Kent's data
($R = 0.1, X/D = 80$)



Turbulent transport of chemical species

The present analysis assumes that the main directions of chemical species transport is in y-axis. Figures 12 and 13 show the transport of fuel, oxidant and product in the y-direction. In Figure 13, it is found that the maximum transport

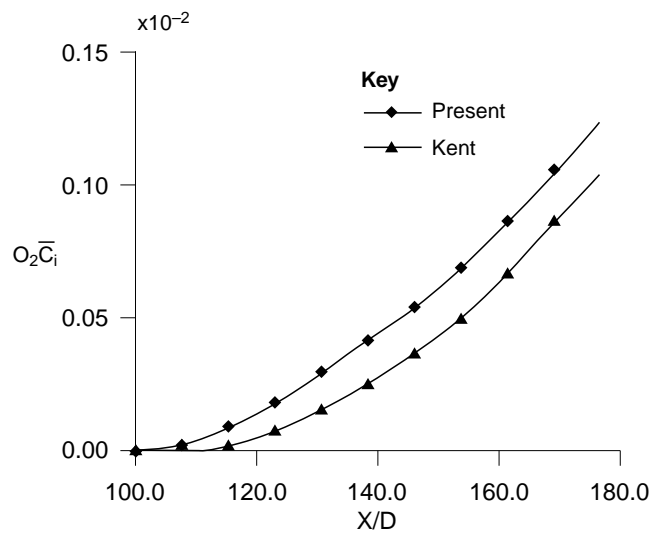


Figure 11. O₂ concentration distributions along centerline compared with Kent's data

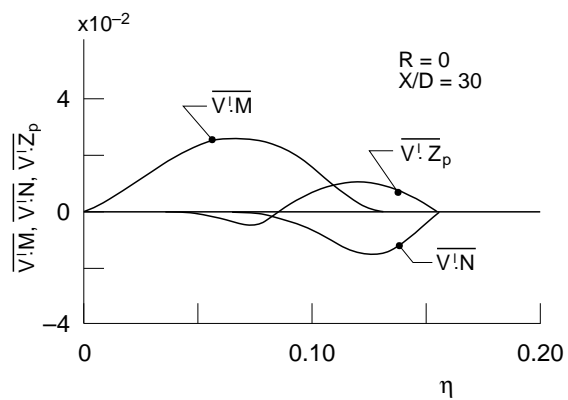


Figure 12. Turbulent transport of species in y-direction (X/D = 30)

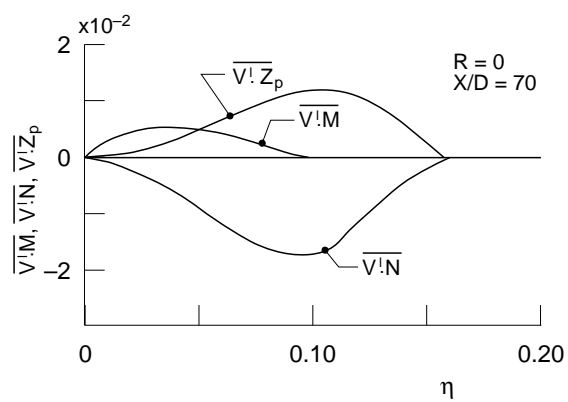


Figure 13. Turbulent transport of species in y-direction (X/D = 70)

of oxidant appears at $\eta = 0.095$, but the result in Figure 8 shows that the maximum slope of oxidant concentration appears at $\eta = 0.11$. Therefore, one can see that the oxidant transport opposes the concentration gradient between $\eta = 0.095$ and 0.11 . This signifies clearly that eddy-transport can not be expressed as a gradient type-transport (i.e. laminar or molecular transport).

Temperature distributions and turbulent heat transfer

The temperature of fuel and air before mixing is assumed to be 300K. The temperature distributions at different cross-sections are shown in Figures 14 and 15. The results are compared with Kent's (Kent and Bilger, 1975) experimental data. Again the trends and general characteristics of the present results are in good agreement with the experimental data. The stoichiometric combustion adiabatic flame temperatures of the fuel used in Kent's experiment and in the present calculation are 2,500K and 2,450K respectively, thus the temperature comparison between the present calculations and Kent's data is reasonable. The temperature distribution of Kent's experiment at the centerline is higher than the present results because the stoichiometric combustion adiabatic flame temperature of fuel used in Kent's experiment is higher, as shown in Figure 14. The temperature distribution of the present results approaches Kent's data at the downstream position of $X/D = 120$ owing to the complete mixing and the same combustion model, as shown in Figure 15.

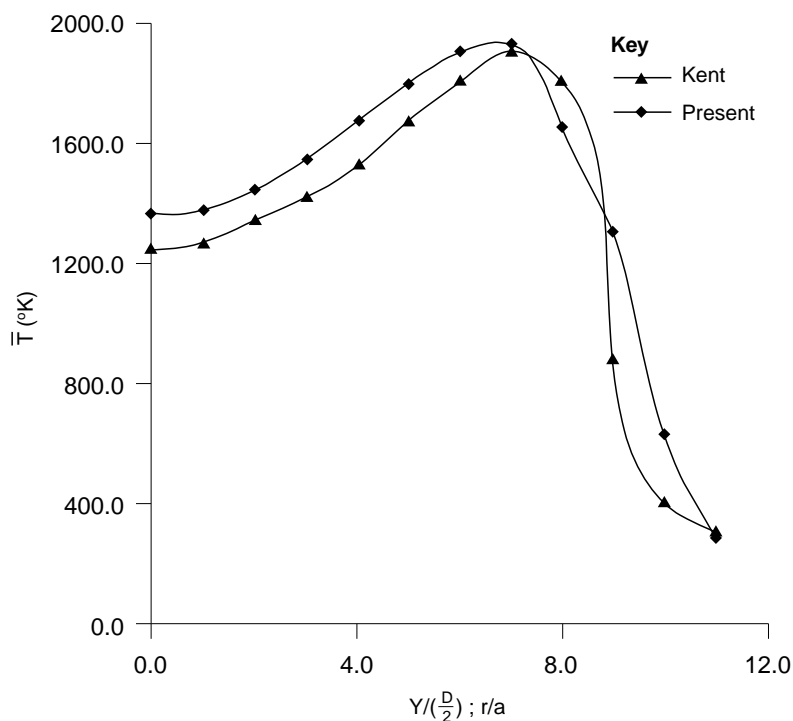


Figure 14.
Temperature distributions compared with Kent's data ($R = 0.1, X/D = 40$)

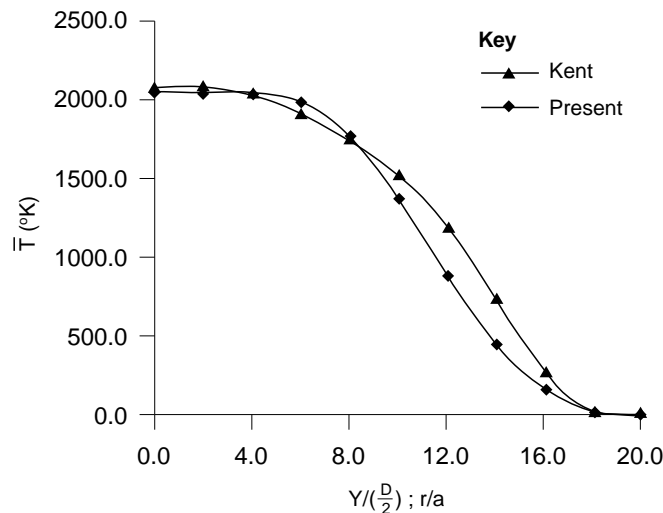


Figure 15.
Temperature
distributions compared
with Kent's data
($R = 0.1$, $X/D = 120$)

Turbulent heat transfer $\langle \nu T' \rangle$ and the corresponding average temperature distributions are shown in Figure 16. In Figure 16(a) the maximum transport of heat for $X/D = 30$ appears at $\eta = 0.05$, but the maximum slope of the mean temperature is at $\eta = 0.07$. This signifies that the turbulent heat transfer $\langle \nu T' \rangle$ opposes the gradient of temperature between $\eta = 0.05$ and 0.07 . This behavior parallels the commonly accepted physical explanation for such turbulent combustion phenomena. Turbulent mixing is an eddy-transport phenomenon in which molecular mixing may not be completed to the degree indicated by the mean profiles.

Flame structure

The flame zone exists between the fuel limit and oxidant limit as shown in Figures 17 and 18. The solutions provide an explanation for the existence of the thick, turbulent diffusion flames even with an infinitely fast reaction rate scheme. The laminar flame sheet results from molecular transport across the adjacent diffusion layer. In the present situation, transfer occurs through velocity space. Only when the reactants are brought into coexistence in velocity space does combustion proceed. The fundamental nature of the solutions confirms that the turbulent flame zone exists (instead of the flame sheet solution). As mentioned above, the velocity ratio influences the length of the flame, and one can find at the same time that the velocity ratio also influences the width of the flame. The maximum temperature line and the temperature influenced zone are also shown in these figures.

Conclusions

A study of turbulent plane jet combustion using the kinetic theory approach of Chung and the Green's function solution of Hong has been presented in this

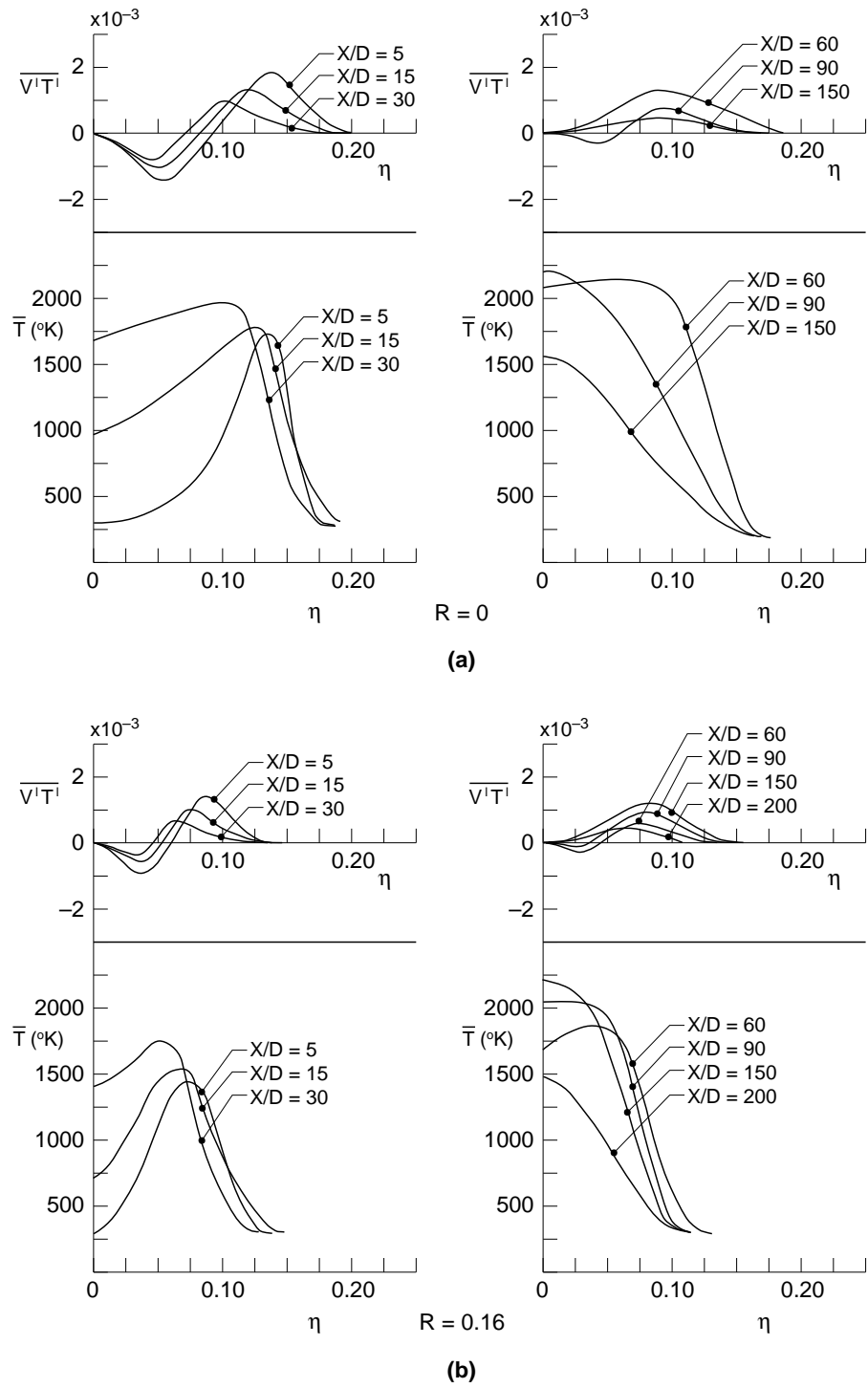


Figure 16.
Turbulent heat transfer
in v' -velocity space and
the mean temperature
distributions

paper. Many physical quantities, such as mass fraction of species, combustion temperature and flame structure have been calculated and good agreement in comparison with the available experimental data has been observed. The detailed dynamic behavior of the reacting process in the turbulent field could be better understood using the real probability density function of the fluid element in velocity space. The present solutions of turbulent heat transfer parallel the concept of eddy-type turbulent transport (rather than gradient-type molecular transport). The governing mechanism of the flame zone within the model for this physical phenomenon is that the reactants are carried by the fluid elements which undergo eddy transport through velocity space. The existence of thick, turbulent diffusion flame structure solutions, even with an infinitely fast reaction rate, confirm the applicability of the present turbulent kinetic theory to engineering problems.

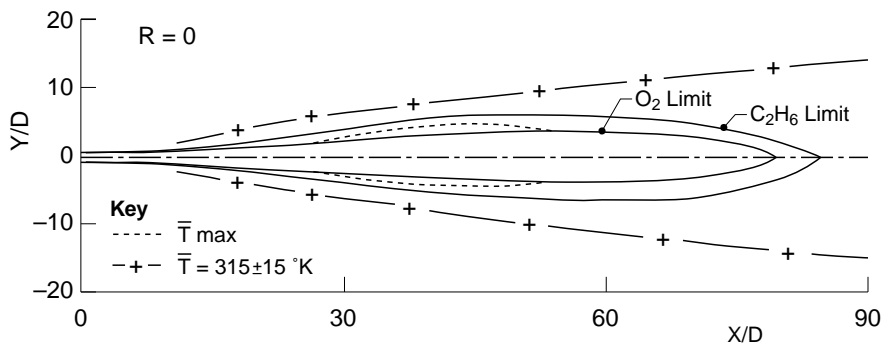


Figure 17.
Flame structure with
 $R = 0.0$

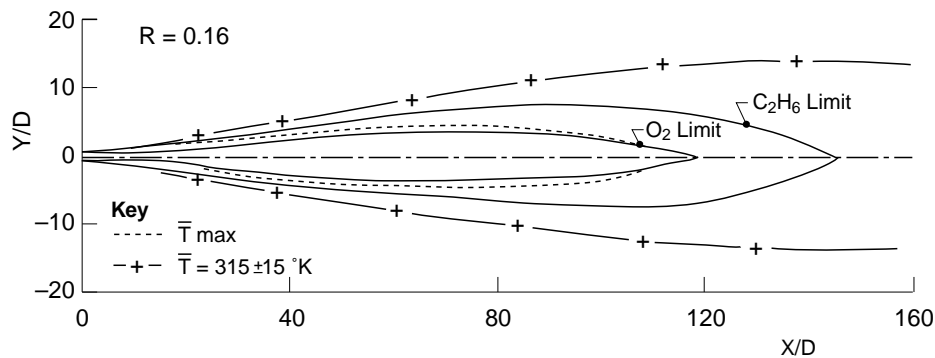


Figure 18.
Flame structure with
 $R = 0.16$

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