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A SIMPLE REACTION-RATE MODEL
FOR TURBULENT DIFFUSION FLAMES

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Abstract

A simple reaction-rate model is proposed for turbulent diffusion flames. This model was derived from the results of Chung (1972), and has reaction rate proportional to turbulence mixing rate. The reaction rate is also dependent on the mean mass fraction and the mean-square fluctuation of mass fraction of each reactant. Calculations are compared with experimental data of Kent and Bilger (1973), and are generally successful in predicting the measured quantities.

Nomenclature

\( a, b, c \) Stoichiometric coefficients of fuel, oxygen, and product, respectively

\( C_i \) mass fraction of specie \( i \); \( c_i \), turbulent fluctuation

\( C_{e1}, C_{e2} \) empirical constants, equal to 1.93 and 1.92, respectively

\( C_{g1}, C_{g2} \) empirical constants, equal to 3.0 and 0.20, respectively

\( C_\mu \) empirical constant, equal to 0.09

\( D \) diameter of hydrogen injector

\( \sigma_i^2 \) mean-square fluctuation of mass fraction, \( \sigma_i^2 \)

\( h \) static enthalpy

\( l_o \) stagnation enthalpy

\( k \) mean turbulence kinetic energy, \( \frac{u_i u_i}{2} \)

\( p \) pressure

\( r \) radial distance from the axis of symmetry

\( U, V \) velocity in \( x, y \) directions

\( u, v \) turbulence velocity in \( x, y \) directions
Introduction

There have been a number of studies directed toward modeling the effect of turbulence on chemical reactions. These studies have been motivated by the need to develop methods for computing turbulent, chemically-reacting flow fields for a wide variety of applications. Spalding proposed three such models¹-³, all for cases where the chemical reaction time is much less than the characteristic time for turbulent mixing. His first model¹ was for
initially unmixed reactants that react instantly on contact. It was assumed that the instantaneous fuel-air ratio at a point was equal to the mean value, plus or minus the root-mean-square fluctuation. For each of these two values, the temperature and composition for complete reaction was computed. Calculations indicated a finite flame width, which is qualitatively correct. This model has not been extensively compared with experiment, however. Spalding's second and third models\(^2,3\) were developed for premixed flames, and were called eddy breakup models. Each had the mean fuel reaction rate proportional to \(\varepsilon/k\), the characteristic mixing rate of the turbulence. The second and third models also had mean fuel reaction rate proportional to mean fuel mass fraction and to root-mean-square fluctuation of fuel mass fraction, respectively. Both of these models have had some success when compared with experimental data for premixed flows.

Rhodes, Harsha and Peters\(^4\) did not use species conservation equations, and so did not model the reaction-rate terms directly. They divided the flow field into classes and zones, characterized by instantaneous and mean concentrations of the fuel, respectively. An assumed probability density for concentration fluctuations was used to develop a model for their effect on mean density. (Correlations involving density fluctuations were neglected, however). This model was combined with both equilibrium chemistry and finite-rate chemistry models. In the latter, each class was assumed to behave as a one-dimensional, transient stirred reactor, Their computations were compared with the data of Kent and Bilger\(^5\) for \(U_j/U_e = 10\).

Hilst, et al\(^6\), developed second-order closure methods for the species continuity equations, and combined these with turbulent diffusion models. These models conformed to the principles of invariant modeling. A limited number of calculations were performed for two-dimensional diffusion and isothermal reaction of two species. Libby\(^7\) considered the equations
describing turbulent reacting flows with fast chemical reactions. Effects of
density fluctuations were included in the formulation. Specific closure models
were not proposed, however.

There have also been a number of studies which considered simplified
flow fields, in an effort to describe the interaction between turbulence and
chemical reactions in greater detail. Among these are Chung, Alber and Batt,
and O'Brien. In these analyses, the probability density functions for
velocity and scalar fluctuations were modeled and used to compute various
correlations. The analysis of Chung formed the basis of the model described
here.

This paper has two purposes. First to propose a simple reaction-rate
model applicable to turbulent diffusion flames; for which the time scale for
chemical reaction is much smaller than the time scale for turbulent mixing.
Second, to provide a limited assessment of the proposed model by comparing
calculations with experimental data.

Reaction-Rate Model

In this section, Chung's analysis of homologous shear flow forms the
basis for a model of the chemical reaction rate in a turbulent flow. It is
assumed that the chemical reaction time is much less than the turbulent mixing
time. Also, it is assumed that the Reynolds number is large and that
solid boundaries have negligible influence, so that molecular transport can be
neglected.

Chung considered a one-dimensional shear flow with nonzero derivatives
in the y-direction, only. He also assumed constant density, so that the
velocity field was not affected by the temperature field. For these conditions,
the mean species conservation equation for the fuel \( f \) is:

\[
\frac{d}{dy} (v_c f) = \frac{v_c}{w_f}
\]  

(1)

In his solution, Chung \(^8\) represented the probability density of the fluid elements by the sum of two half-Maxwellian functions containing a total of four parameters. A moment method was used to solve for these parameters. These in turn determined mean velocity gradient, turbulence energy, and Reynolds stress.

Next, consider that the combustion is described by the following one-step chemical reaction:

\[
a (\text{fuel}) + b (\text{oxidizer}) \rightarrow d (\text{product})
\]  

(2)

Chung's \(^8\) solution for the probability densities, when the chemical reaction time is much smaller than the turbulent mixing time, allows the correlation \( \overline{vc_f} \) to be evaluated. It is:

\[
\overline{vc_f} = \left[ (1 - \pi/\delta k/3\pi) \right]^{0.5} c_f
\]  

(3)

In the combustion region, the solution for \( c_f \) is linear in \( y \). Although Chung did not explicitly do so, an equation for \( \overline{\dot{w}_f} \) can be obtained by substituting (3) and the solution for \( c_f \) into (1). After some manipulation, the result can be expressed as:

\[
\overline{\dot{w}_f} = - (3/\delta \pi) \left( k^{0.5}/\lambda \right) \left[ \overline{c_f} + g_f^{0.5} + (\overline{w_f}/\overline{w_o}) (\overline{c_o} + g_o^{0.5}) \right]
\]  

(4)

where \( \lambda \) is the local integral scale of the turbulence. In (4), the rate
\( k^{0.5/\ell} \) is consistent with the condition that turbulent motion controls the reaction rate. The quantity in brackets provides an estimate of the effect of the amount of each reactant on the reaction rate.

It is here hypothesized that (4) is approximately valid at each point in more complex flows than the one-dimensional shear flow considered by Chung. This hypothesis was incorporated into a calculation method that uses differential equations for \( k \) and \( \epsilon \) to describe turbulence transport. If the estimate \( \epsilon = k^{1.5/\ell} \) is made, (4) can be written in terms of \( k \) and \( \epsilon \) as:

\[
\overline{w_f} = -A(e/k) \left[ \overline{c_f} + g_f^{0.5} + (\overline{w_f}/\overline{w_o}) (\overline{c_o} + g_o^{0.5}) \right]
\]  

(5)

where \( A \) is about 0.17. Comparisons with experimental data, to be discussed in the next section, suggest that \( A = 0.22 \) is a better estimate.

The dependence of \( \overline{w_f} \) on mass fraction resembles a result derived by Gibson and Libby for steady flow relative to a reaction zone, with oxidizer and product on one side and fuel and product on the other. Their solution has \( c_f^{(\infty)} \) instead of \( \overline{c_f} + g_f^{0.5} \), and \( c_o^{(\infty)} \) instead of \( \overline{c_o} + g_o^{0.5} \). Here \( c_f^{(\infty)} \) and \( c_o^{(\infty)} \) are the mass fractions of fuel and oxidizer in the volumes adjacent to the reaction zone. Following Gibson and Libby, (5) may perhaps be interpreted as a mean rate of consumption of fuel at a point, related to the frequency of passage of reaction zones through that point. Equation (5) is also related to Spalding's models for premixed flames, in that \( \overline{w_f} \) is proportional to \( e/k \). The dependence on amount of reactants is different, however. It is evident that \( \overline{w_f} \) as calculated by (5) does not go to zero when one of the reactants disappears. For this reason \( \overline{w_f} \) was set equal to zero when the sum of the mean value and the root-mean-square fluctuation of
mass fraction of either reactant was less than $10^{-4}$.

The differential equations for $g_f$ and $g_o$ also contain reaction rate
terms, $c_f \rho \dot{w}_f$ and $c_o \rho \dot{w}_o$, respectively. For the one-dimensional
shear flow studied by Chung, the species conservation equation for fuel can
be written, after multiplying by $C_f$ and taking the time average, as:

$$\frac{d}{dy} \left( \nu C_f^2 / 2 \right) = C_f \dot{w}_f$$

(6)

Using Chung's solution for the probability densities to evaluate $\nu C_f^2$
gives:

$$C_f \dot{w}_f = (\delta_f + \delta_f^{0.5}) \dot{w}_f$$

so that $C_f \dot{w}_f = \delta_f^{0.5} \dot{w}_f$. This can be used in the equation for $g_f$ by
neglecting density fluctuations, giving $C_f \rho \dot{w}_f = \rho g_f^{0.5} \dot{w}_f$.

Summary of Equations

The following is a summary of the mean differential equations that
were solved. They are written for axially symmetric flow in the boundary-
layer approximation. Density fluctuations have been neglected. Various
turbulence transport terms have been modeled as described by Lauder and
Spalding. The conservation equations are:

Mass:

$$\partial (\bar{\rho} \bar{u}_r)/\partial x + \partial (\bar{\rho} \bar{v}_r)/\partial r = 0$$

(7)

x-momentum:

$$\bar{\rho} \bar{u} \partial \bar{u}/\partial x + \bar{\rho} \bar{v} \partial \bar{u}/\partial r = r^{-1}(\partial/\partial r)(r \mu_T \partial \bar{u}/\partial r) - \partial \bar{p}/\partial x$$

(8)
where
\[ \mu_T = c_\mu \bar{p} k^2 / \epsilon \]  \hspace{1cm} (9)

Energy:
\[ \bar{p} \bar{U} \delta h_o / \delta x + \bar{p} \bar{V} \delta h_o / \delta r = r^{-1}(\delta / \delta r) \left[ r(\mu_T / \sigma_p) \delta h / \delta r \right] + r \mu_T \bar{U} \delta u / \delta r \]

where
\[ \delta h_o = \delta h + \frac{1}{2} \bar{u}^2 + k \]

Fuel:
\[ \bar{p} \bar{U} \delta c_f / \delta x + \bar{p} \bar{V} \delta c_f / \delta r = \]
\[ r^{-1}(\delta / \delta r) \left[ r(\mu_T / \sigma_f) \delta c_f / \delta r \right] + \bar{p} \bar{V} \]

Reaction invariant:
\[ \bar{p} \bar{U} \delta c_f / \delta x + \bar{p} \bar{V} \delta c_f / \delta r = \]
\[ r^{-1}(\delta / \delta r) \left[ r(\mu_T / \sigma_f) \delta c_f / \delta r \right] \]

where
\[ \delta c_f = \delta f - (W_o b / \bar{W}_f) \delta f_r \]

Fuel fluctuations:
\[ \bar{p} \bar{U} \delta g_f / \delta x + \bar{p} \bar{V} \delta g_f / \delta r = \]
\[ r^{-1}(\delta / \delta r) \left[ r(\mu_T / \sigma_f) \delta g_f / \delta r \right] \] +
\[ c_{g l} \mu_T (\delta c_f / \delta r)^2 - c_{g 2} \bar{p}^2 k \delta c_f / \mu_T + 2 \bar{p} g_f \bar{W} f \bar{W} f \]

The equation for oxygen fluctuations is the same as (13), but with \( g_f, \delta f_r, \) and \( \bar{W}_f \) replaced by \( \delta g_o, \delta o_r, \) and \( \bar{W}_o \), respectively. Here, \( \bar{W}_o \)
equals \( (W_o b / \bar{W}_f a) \bar{W}_f \).

Turbulence kinetic energy:
\[ \bar{p} \bar{U} \delta k / \delta x + \bar{p} \bar{V} \delta k / \delta r = \]
\[ r^{-1}(\delta / \delta r) \left[ r(\mu_T / \sigma_k) \delta k / \delta r \right] \] +
\[ \mu_T (\delta u / \delta r)^2 - \bar{p} \epsilon \]
Turbulence dissipation rate:

\[
\begin{align*}
\bar{p} \frac{\partial \bar{e}}{\partial \bar{x}} + \bar{p} \frac{\partial \bar{e}}{\partial \bar{r}} &= r^{-1} \left( \frac{\partial}{\partial \bar{r}} \right) \left[ r \left( \mu_0/\sigma_e \right) \frac{\partial \bar{e}}{\partial \bar{r}} \right] \\
&+ c_{e1} \left( \varepsilon/k \right) \mu_0 \left( \delta \bar{u}/\delta \bar{r} \right)^2 - c_{e2} \bar{p} \varepsilon^2/k
\end{align*}
\]

There is also a differential equation for \( \bar{c}_N \), of the same form as (12). These differential equations were supplemented by equations of state, which assume a mixture of perfect gases with variable specific heats. The numerical solution was performed using a finite-difference method based on that of Patankar and Spalding.16

Comparisons with Experiment

A limited evaluation of this reaction-rate model has been made by comparing calculations with the experimental data of Kent and Bilger5 for velocity ratios \( \bar{U}_j/\bar{U}_e \) equal to 10, 5, and 2. These experiments were chosen as a standard of comparison because of the extensive flow field measurements, including initial conditions for \( \bar{u}^2 \). The experimental arrangement was a central hydrogen jet issuing into a parallel, coaxial air stream. Both streams were subsonic and initially at about 300K. There was a slight favorable pressure gradient, caused by the influence of the tunnel walls.

The initial conditions and the pressure gradient for the calculations were the same as those measured5. \( k \) and \( \varepsilon \) were not measured directly, however. The initial values of \( k \) were determined by \( k = \bar{u}^2/4 \mu_0 c_{0.1} \), based on conditions in the inertial sublayer of a boundary layer14. Initial values of \( \varepsilon \) were determined from \( k \) and the measured \( \bar{U}(y) \) through the approximation \( \varepsilon = c_{0.5} k \delta \bar{u}/\delta \bar{r} \). This was based on the approximation that
Reynold stress is proportional to $k$, and on (9). Initial conditions for $\varepsilon_f$ were assumed to be $\varepsilon_f = 2\varepsilon(\frac{\partial}{\partial t})^2$, and similarly for $\varepsilon_g$.

The most extensive set of measurements reported by Kent and Bilger were for $\bar{U}_f/\bar{U}_e = 10$. In making calculations for this case, a number of values of the coefficient $A$ in (5) were tried. The value 0.22 gave somewhat better comparison with experiment than the original estimate of 0.17. Figures 1-7 show comparisons of calculations using $A = 0.22$ with experiments for $\bar{U}_f/\bar{U}_e = 10$. Figure 1 shows the axial variation of centerline values of temperature and of mole fraction of $H_2$, $O_2$, and $H_2O$. Figures 2-5 show radial profiles of these four quantities at $x/D$ of 40, 80, 120, and 160. These comparisons show satisfactory agreement overall, and are generally best nearer the injector (smaller $x/D$) and closer to the centerline (smaller $r/r_f$). The latter may be related to the omission from the analysis of intermittency effects. Also, the omission of correlations involving density fluctuations is expected to be important at larger $r/r_f$, where there are large density gradients. Figures 3 and 5 also show results calculated by Rhodes, et al, using an integral method, with equilibrium chemistry and their model for the mean density. At $x/D = 80$ (Figure 3), the present method and that of Rhodes, et al, are both in good agreement with experiment. At $x/D = 160$ (Figure 5), however, the results of the present method are in substantially better agreement with experiment.

Figure 6 shows flame contours. The $H_2$ and $O_2$ limits are where the mole fractions of $H_2$ and $O_2$ are 0.01 and 0.005, respectively. The stoichiometric line is where $H_2$ and $O_2$ appear in stoichiometric proportions. If the intersection of the stoichiometric line with the axis is used as a measure of flame length, then the calculation overpredicts this case by about
7%. Turbulence levels on the axis are shown in Figure 7. The calculated line is based on the assumption that \( \sqrt{v^2} \) equals \((2/3)k\), as for isotropic turbulence.

Calculations were also made for \( \bar{U}_j/\bar{U}_e \) of 5 and 2 using \( A \) equal to 0.22. Figure 8 shows the axial variation of temperature and of mole fractions of \( H_2, O_2, \) and \( H_2O \) for \( \bar{U}_j/\bar{U}_e = 5 \). Radial profiles of these quantities at \( x/D \) of 40 are shown in Figure 9. The same information for \( \bar{U}_j/\bar{U}_e = 2 \) is shown in Figures 10 and 11. These comparisons show rather close agreement with experiment, as for \( \bar{U}_j/\bar{U}_e = 10 \). This lends some support to the idea that the coefficient \( A \) is nearly a constant, although this is not conclusive. Again there is generally better agreement for smaller \( x/D \) and smaller \( r/r_j \).

The axial variation of mean velocity for all three velocity ratios is compared with experiment in Figure 12. For \( \bar{U}_j/\bar{U}_e \) of 10 and 5, calculations are within about 5% of experiment. Differences of up to 16% occur for \( \bar{U}_j/\bar{U}_e = 2 \), however. This may be a result of the turbulence transport model, because when the velocity excess in the jet is small, the model predicts a velocity decay rate that is slower than measured\(^{17}\). This applies for \( \bar{U}_j/\bar{U}_e = 2 \), where for example at \( x/D = 80 \), the calculation gave \( \bar{U}_c/\bar{U}_e = 1.052 \).

Although the reaction-rate model proposed here greatly simplifies the actual physical behavior, this model and the turbulence transport model\(^{12,13}\) were generally successful in predicting measured values from the experiments of Kent and Bilger\(^5\). The favorable results obtained so far, plus the ease of use of the model, justify further consideration of this reaction-rate model for turbulent diffusion flame calculations.
Summary

The simple reaction-rate model for turbulent diffusion flames proposed here has the following major characteristics: (1) the reaction rate is proportional to the turbulence mixing rate; (2) the reaction rate is dependent on the mean mass fraction and on the mean square fluctuation of mass fraction of each reactant.

Computations using this reaction-rate model have been generally successful in predicting measured quantities for three hydrogen jet to air stream velocity ratios from the experiments of Kent and Bilger\(^5\).

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