PROGRESS IN THE DEVELOPMENT OF PDF TURBULENCE MODELS FOR COMBUSTION

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I. Introduction

(U) A combined Monte Carlo—CFD algorithm has been developed recently at NASA lewis Research Center for turbulent reacting flows. In this algorithm, conventional CFD schemes are employed to obtain the velocity field and other velocity related turbulent quantities, and a Monte Carlo scheme is used to solve the evolution equation for the probability density function (pdf) of species mass fraction and temperature.

(U) In combustion computations, the predictions of chemical reaction rates (the source terms in the species conservation equations) are poor if conventional turbulence models are used. The main difficulty lies in the fact that the reaction rate is highly non-linear, and the use of averaged temperature produces excessively large errors. Moment closure models for the source terms have attained only limited success. The probability density function (pdf) method seems to be the only alternative at the present time that uses local instantaneous values of the temperature, density, etc., in predicting chemical reaction rates, and thus may be the only viable approach for more accurate turbulent combustion calculations. The closure problem and the need for pdf has been discussed in detail in a previous paper[1].

(U) Assumed pdf are useful in simple problems; however, for more general combustion problems, the solution of a evolution equation for the pdf is necessary.

II. Method

(U) Conventional CFD flow solvers are quite common and needed no explanation here. We will concentrate on the derivation and solution of the pdf evolution equation in this section.

2.1 PDF evolution equation of mass fraction.

(U) For simplicity, the pdf equation for a single scalar will be derived here. The extension to multi species is trivial. The species transport equations (for a single species) can be written as

$$\rho\partial_t Y = -\rho u_k \partial_k Y + \rho\partial_k(D\partial_k Y) + \rho w \qquad (0.1)$$

where u_k is the velocity, Y is the mass fraction, and w is the chemical source term; summation for repeated indices is understood.

Let $P(Y)$ be the probability density function, and define $\phi = exp(i\lambda c)$, then the characteristic function of the pdf can be written as the ensemble average of ϕ:

$$< \phi >= \int P(Y)\phi dY,$$

and the pdf can be written as the inverse Fourier transform of the characteristic function:

$$P(Y) = \frac{1}{2\pi}\int < \phi > exp(-i\lambda Y)dY.$$

Now differentiate ϕ with respect to time,

$$\partial_t \phi = i\lambda exp(i\lambda Y)(\partial_t Y),$$

and replace $\partial_t Y$ in the above equation with the right hand side of eq. (1), we obtain

$$\rho\partial_t\phi = i\lambda exp(i\lambda Y)[-\rho u_k \partial_k Y + \partial_k(\rho D\partial_k Y) + \rho w],$$

which can be rearranged as

$$\partial_t(\rho\phi) + \partial_k(\rho u_k \phi) = i\lambda\phi\partial_k(\rho D\partial_k Y) + i\lambda\phi\rho w$$

Take ensemble average of the above equation gives

$$\partial_t < \rho\phi > +\partial_k < \rho u_k\phi >= i\lambda < \rho w\phi > +i\lambda < \phi\partial_k(\rho D\partial_k Y) > .$$

The inverse Fourier transform of the above equation gives the evolution equation for the probability density function:

$$\begin{aligned} &\partial_t(\rho P) + \partial_k(\rho < u_k > P) + \partial_Y(\rho w P) \\ &= -\partial_k(\rho < u_k' | Y > P) - \partial_Y(< \partial_k(\rho D\partial_k Y) | Y > P) \end{aligned}$$

where the terms represent mean convection, chemical reactions, turbulent convection, and molecular mixing, respectively.

For multi species and temperature, the pdf is written as $P(\psi_1, ..., \psi_n)$, where $\psi_i, i = 1, ..., n$ represent the scalars including mass fractions and temperature. A similar derivation gives

$$\begin{aligned} &\bar{\rho}\partial_t P + \bar{\rho}\bar{v}_\alpha\partial_\alpha P + \bar{\rho}\sum_{i=1}^{N}\partial_{\psi_i}\{w_i(\psi_1, ..., \psi_N)P\} \\ &= -\partial_\alpha(\bar{\rho} < v_\alpha'' | \psi_i > P) - \bar{\rho}\sum_{i=1}^{N}\sum_{j=1}^{N}\partial^2_{\psi_i\psi_j}(< \epsilon_{ij} | \psi_k > P). \end{aligned}$$

(U) The left hand side of the above equation can be evaluated exactly and requires no modeling; the right hand side terms contain the conditional average of the Favre velocity fluctuation and the conditional average of the scalar dissipation and require modeling.

2.2 Modeled pdf equation

(U) The first term that needs modeling is the turbulent diffusion term, for which the following gradient model is used:

$$- < u_k'|\psi_i > P \cong D_t \partial_\alpha P,$$

where D_t is the turbulent diffusion coefficient, which is set to be equal to the eddy viscosity, i.e., the turbulent Schmidt number is equal to one.

(U) The next term needs modeling is the molecular mixing term. A coalescence/dispersion model is used for this term, which has the following general form:

$$\begin{aligned} & -\bar{\rho} \sum_{i=1}^{N} \sum_{j=1}^{N} \partial^2_{\psi_i \psi_j} (< \epsilon_{ij} | \psi_k > P) \\ \cong & \frac{C_D}{\tau} \int \int P(\psi') P(\psi'') T(\psi | \phi', \psi'') d\psi' d\psi'' - P \\ & \equiv D_m P \end{aligned}$$

where T is the transition probability. For more detail description of the molecular mixing model, see Ref 2. The modeled the pdf equation is then

$$\begin{aligned} & \bar{\rho} \partial_t P + \bar{\rho} \bar{v}_\alpha \partial_\alpha P + \bar{\rho} \sum_{i=1}^{N} \partial_{\psi_i} \{ w_i(\psi_1, ..., \psi_N) P \} \\ & = \partial_j (D_t \partial_\alpha P) + D_m P \end{aligned}$$

2.3 Solution of the pdf equation

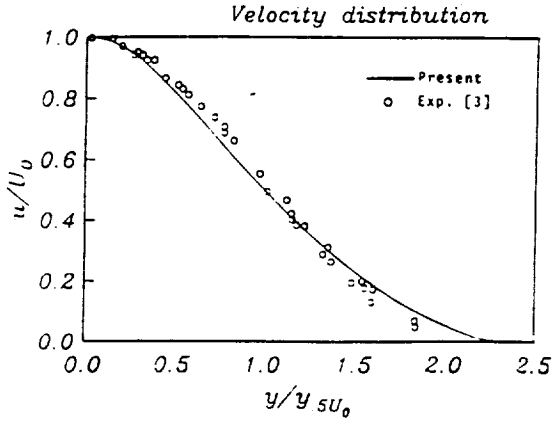
(U) A fractional step method is used to solve the pdf equation in a Monte Carlo simulation. Three processes, namely, (1) convection/diffusion, (2) molecular mixing, and (3) chemical reaction, are simulated consecutively:

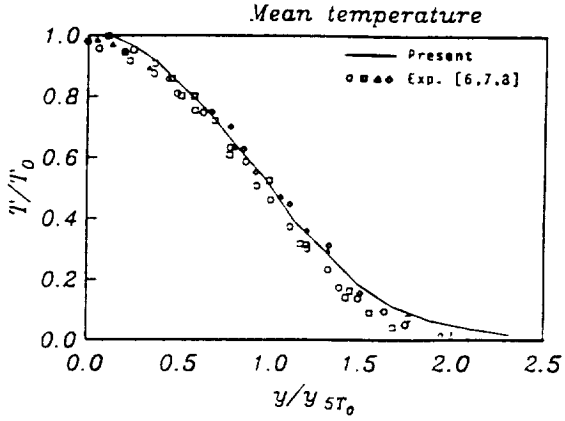
$$(\partial_t + \bar{\rho} \sum_{i=1}^{N} \partial_{\psi_i} \{ w_i(\psi_1, ..., \psi_N) \}) (\partial_t - D_m)(\partial_t + \bar{\rho} \bar{v} \partial_\alpha - \partial_\alpha (D_t \partial_\alpha) P = 0.$$

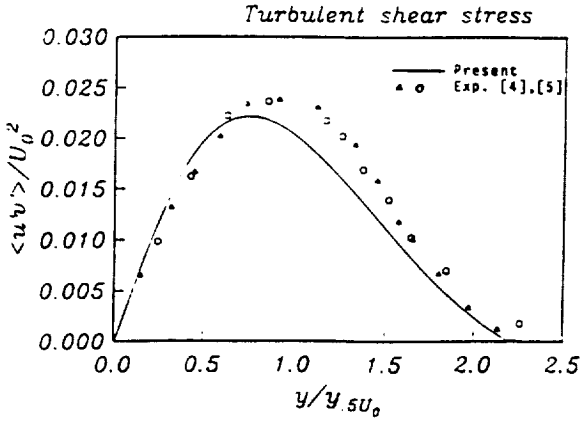
This equation is solved using a Monte Carlo simulation, i.e., the pdf is represented by an ensemble of samples. These sample points move in the hyperspace of $(x_1, x_2, x_3, \psi_1, ..., \psi_n)$ according to the above equation.

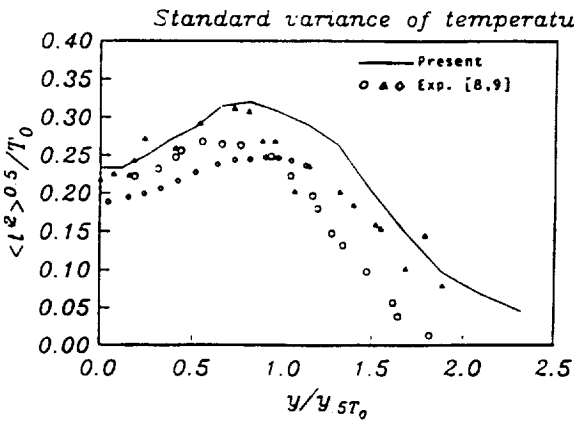
III. Results

(U) A heated turbulent plane jet had been calculated and results reported at last NASP symposium. The case has since been recalculated using modified turbulence model, and improved results are shown here.

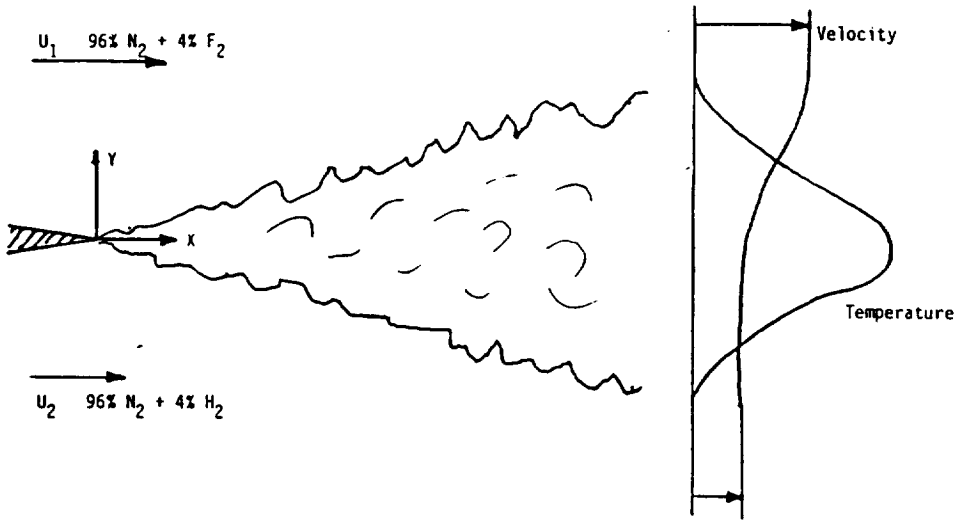


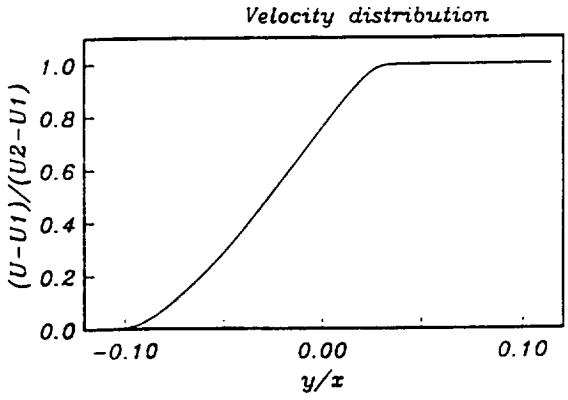


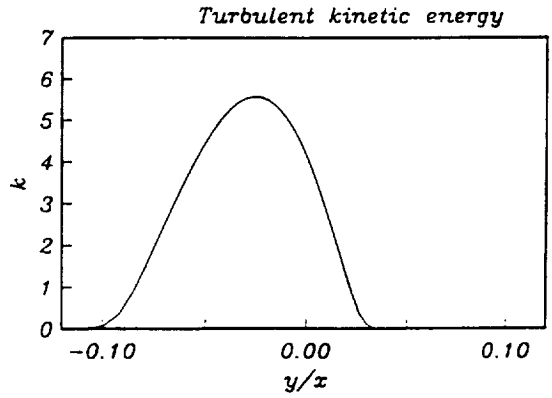




(U) A hydrogen-fluorine diffusion flame was calculated. The flowfield and flow conditions, as well as the calculated velocity and turbulent kinetic energy distribution, are given on this page.







(U) Figures show the calculated heat release of the H2-F2 flame (temperature distribution) compared to experimental data, and the species mass fraction from pdf calculation.

Fig.1 Temperature distribution: H2+F2=2HF

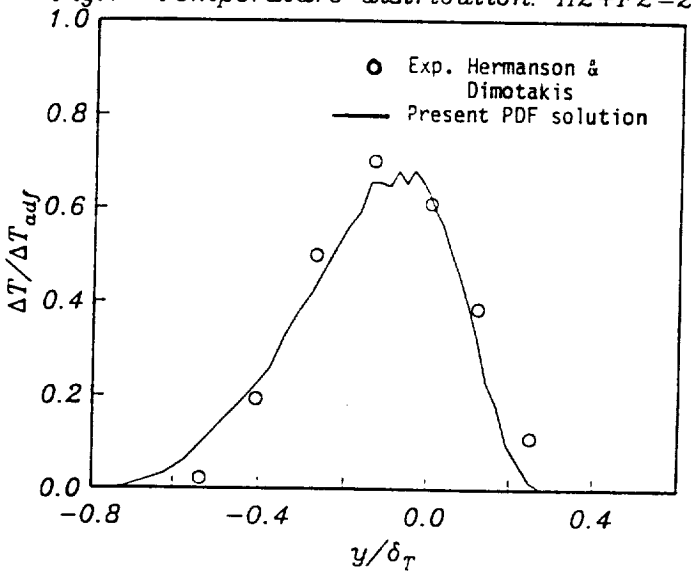
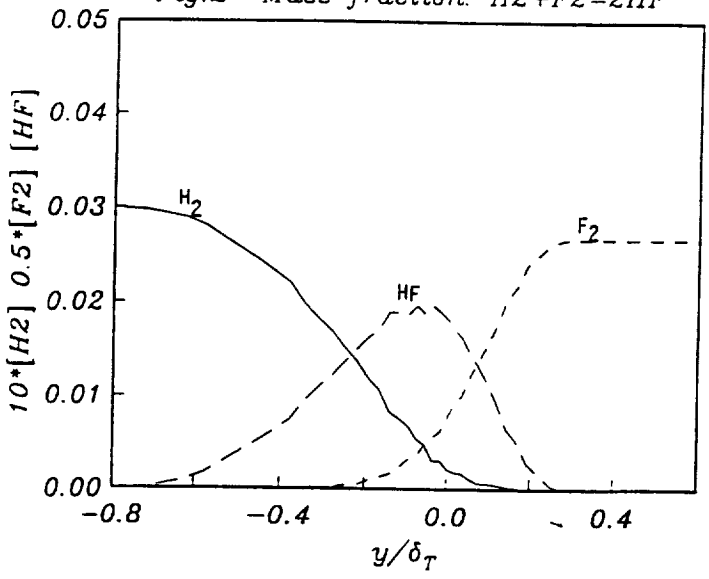


Fig.2 Mass fraction: H2+F2=2HF



(U) Computed pdf of temperature distribution in the H2-F2 flame.

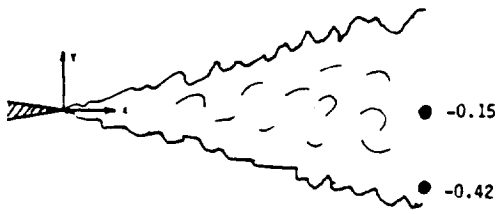
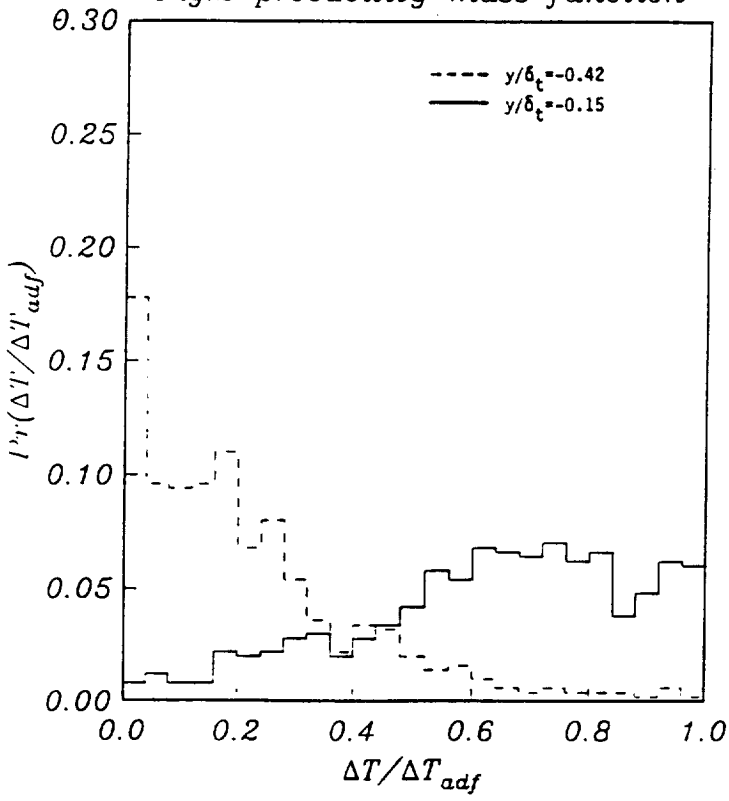


Fig.2 probability mass function



Acknowledgement

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