THE STUDY OF PDF TURBULENCE MODELS IN COMBUSTION

Andrew T. Hsu
Sverdrup Technology, Inc.
& Center for Turbulence Modeling
NASA Lewis Research Center
Cleveland, Ohio

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I. Introduction

(U) In combustion computations, it is well known that 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, pressure and density 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 is the only viable approach for more accurate turbulent combustion calculations.

(U) The fact that the pdf equation has a very large dimensionality renders finite difference schemes extremely demanding on computer memories and thus impractical, if not entirely impossible. A logical alternative is the Monte Carlo scheme, which has been used extensively in statistical physics. The evolution equations for the joint pdf of the velocity and species mass fraction have been successfully solved using Monte Carlo schemes, see, e.g., Pope[1]. However, since CFD has reached a certain degree of maturity as well as acceptance, it seems, at least from the stand point of practical applications, that the use of a combined CFD and Monte Carlo scheme is more beneficial. Therefore, in the present study a scheme is chosen that uses a conventional CFD flow solver in calculating the flowfield properties such as velocity, pressure, etc., while the chemical reaction part is solved using a Monte Carlo scheme.

(U) A combined CFD-Monte Carlo computer algorithm has been developed recently. As a first calibration of the Monte Carlo solver recently developed in this work, the discharge of a heated turbulent plane jet into quiescent air is studied. Experimental data for this problem shows that when the temperature difference between the jet and the surrounding air is small, buoyancy effects can be neglected and the temperature can be treated as a passive scalar. The fact that jet flows have a self-similar solution lends convenience in the modeling study. Furthermore, the existence of experimental data for turbulent shear stress and temperature variance (temperature fluctuation) make the case ideal for the testing of pdf models wherein these

values can be directly evaluated.

(U) The following section presents the methodologies used in this study, and a discussion on the numerical results and their comparison with experimental data follows.

II. Method

2.1 Governing equations

(U) The Favre averaged momentum and species transport equations can be written as

$$\bar{\rho}\partial_t\tilde{u}_i + \bar{\rho}\tilde{u}_j\partial_j\tilde{u}_i = -\partial_i\bar{p} + \nu\partial_j\tau_{ij} - \partial_j\widetilde{u_i''u_j''}$$

$$\bar{\rho}\partial_t\tilde{Y}_i + \bar{\rho}\tilde{u}_j\partial_j\tilde{Y}_i = \bar{\rho}\partial_j(D\partial_j\tilde{Y}_i - \widetilde{Y_i''u_j''}) + \partial_j(D\partial_j\bar{\rho}\widetilde{Y_i''}) + \rho\bar{w}_i$$

where u_i is the velocity and Y_i is the mass fraction. The major problem encountered in the numerical study of turbulent combustion lies in the modeling of the chemical source term, $\rho\bar{w}_i$, known as the chemistry closure problem. The Source term w_i is an exponential function of temperature, and it is well know that the use of averaged temperature, $\bar{T}$, in evaluating $\rho\bar{w}_i$ can cause egregious errors. Therefore the accurate prediction of turbulent combustion using conventional turbulence models becomes very difficult. This motivated the use of pdf methods. If the pdf, P, is given, then the mean of the source term can be evaluated exactly:

$$\rho\bar{w}_i = \int\cdots\int \rho w_i(Y_1,...,Y_n,T,\rho)P(Y_1,...,Y_n,T,\rho)dY_1...dY_ndTd\rho$$

To solve for the pdf, we need the following:

2.2 Evolution equation for the pdf

(U) The evolution equation for the probability density function of the mass fractions, temperature, and density, $P(Y_1,...,Y_n,T,\rho)$, can be written as[1]

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

$$= -\partial_\alpha(\bar{\rho} < v_\alpha''|\psi_i > \tilde{P}) - \bar{\rho}\sum_{i=1}^{N}\sum_{j=1}^{N}\partial^2_{\psi_i\psi_j}(< \epsilon_{ij}|\psi_k > \tilde{P})$$

where the terms represent mean convection, chemical reactions, turbulent convection, and molecular mixing, respectively; $\tilde{P}$ is the density-weighted joint pdf:

$$\tilde{P} = \rho P,$$

ϵ is the scalar dissipation:

$$\epsilon_{ij} = -\rho D_{ij} \partial_j Y_i,$$

ψ_i's are variables such as the mass fractions, density, and temperature, and $<,>$ denotes the mathematical expectation of a function.

(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.

2.3 Finite difference solution for the NS equations

(U) In order to simplify the problem so as to concentrate on the study of the pdf models, we have confined our numerical procedures to parabolic flows. A parabolic NS solver with a $k - \epsilon$ turbulence model has been developed. The $k - \epsilon$ model has been tested by solving standard cases such as flat plate boundary layers and free shear layers with satisfactory numerical results.

2.4 Monte Carlo scheme for the pdf equation

(U) A grid dependent Monte Carlo scheme has been employed, primarily following Chen and Kollmann[5]. The task here is to construct an ensemble of sample points, each sample has its own distinct properties such as temperature, mass fraction, etc.: these properties change with time or location such that the probability function of the ensemble evolves according to the evolution equation. Consequently, the pdf of the ensemble is the desired approximate solution for the pdf equation.

(U) Suppose N samples are assigned to a grid cell in the flow domain, the pdf for the ensemble of N samples can then be written as

$$\tilde{P}^*(\psi) = \frac{1}{N} \sum_{j=1}^{N} \delta(\psi - \phi_j)$$

where ϕ_j is the scalar function value carried by the j^{th} sample, e.g., the mass fractions, etc.

(U) In order to have the pdf $\tilde{P}^*$ evolve according to the pdf evolution equation, we discretize the equation on a given grid and write, for parabolic flows:

$$\tilde{P}^*_{x+dx,j} = \alpha_j \tilde{P}^*_{x,j+1} + \beta_j \tilde{P}^*_{x,j} + \gamma_j \tilde{P}^*_{x,j-1}$$

and require

$$\alpha_j + \beta_j + \gamma_j = 1$$

2.5 Recontamination in a Monte Carlo scheme

(U) Using a very simple test case of a convection/diffusion process with two scalars, it was found that the previous scheme[5] does not conserve mass fractions due to re-contamination. It is found that in order to conserve the mass fractions absolutely, one needs to add further restriction to the scheme, namely

$$\alpha_j + \gamma_j = \alpha_{j-1} + \gamma_{j+1} \qquad (*)$$

A new computer algorithm was devised and tested. This algorithm uses a few extra arrays to store informations form the previous time level and thus eliminates the repetition in the sampling process. With the simple test case of two scalars with assumed constant coefficients in the pdf equation, the new algorithm is shown to conserve the mass fractions perfectly. Deficiencies such as directional bias and re-contamination that were found in the previous algorithm are completely eliminated.

(U) It is not yet known whether one can indeed devise a scheme that satisfies relation (*) in general flows, where the coefficients of the pdf equation are variable and are calculated from the flow velocities, turbulence time scale, etc.

III. Results

(U) The sketch of a heated plane jet is given on this page. The flow domain is divided into 30 cells in the cross direction, and 100 samples are assigned to each cell. The numerical results from the present study are compared with experimental data in the following figures.

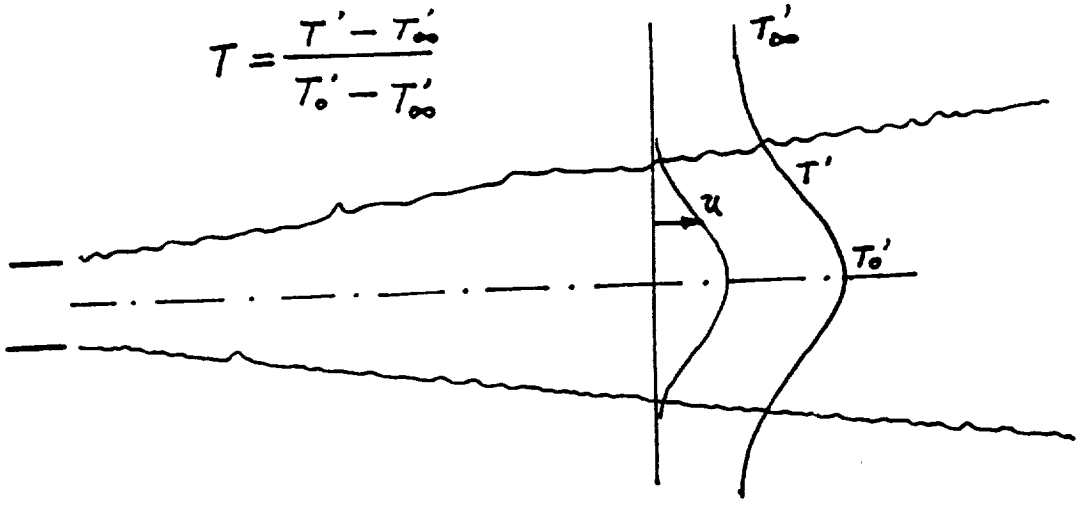
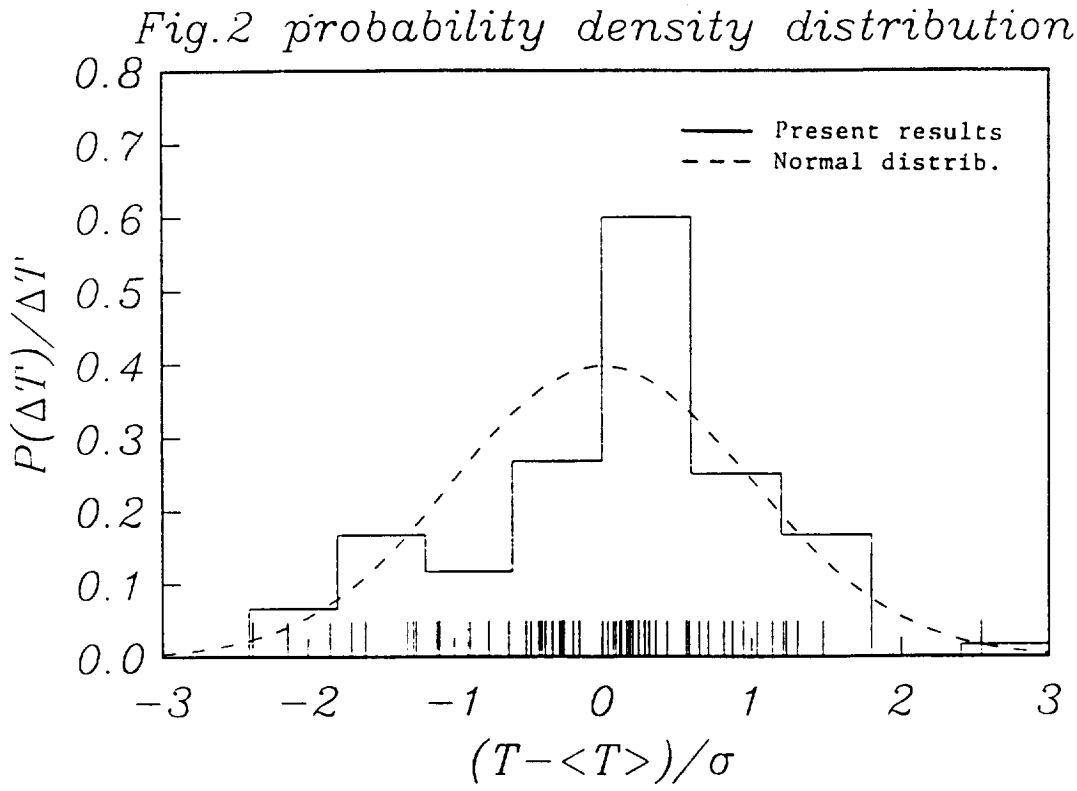
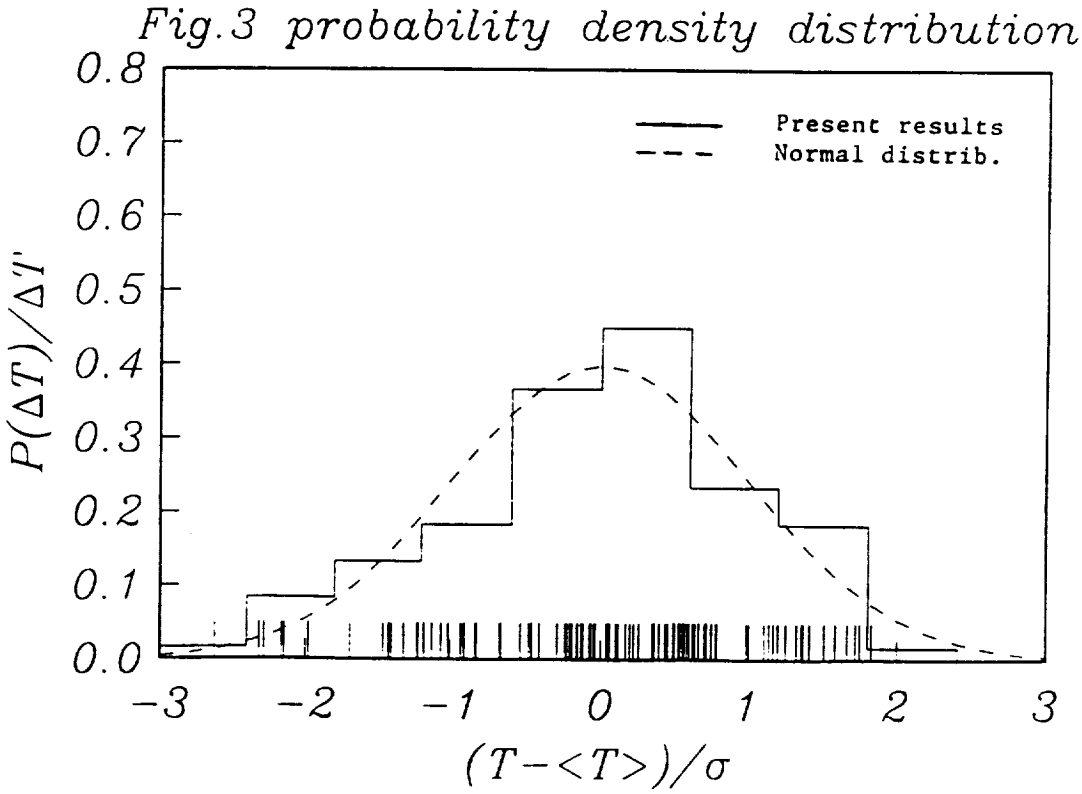


Figure 1. Sketch of a heated turbulent free jet.

(U) The numerical solution for the ensemble averaged pdf's of the temperature: $y/y_{0.5} = 0.$ where $y_{0.5}$ is the location where $T = 0.5T_0$. In order to interpret the data, the ensemble averaged pdfs are integrated to obtain the approximate continuous pdf: $P = P^*(\Delta T)/\Delta T$. The result of this integration is shown as vertical bars. The normal distribution is plotted as a dotted line for comparison.

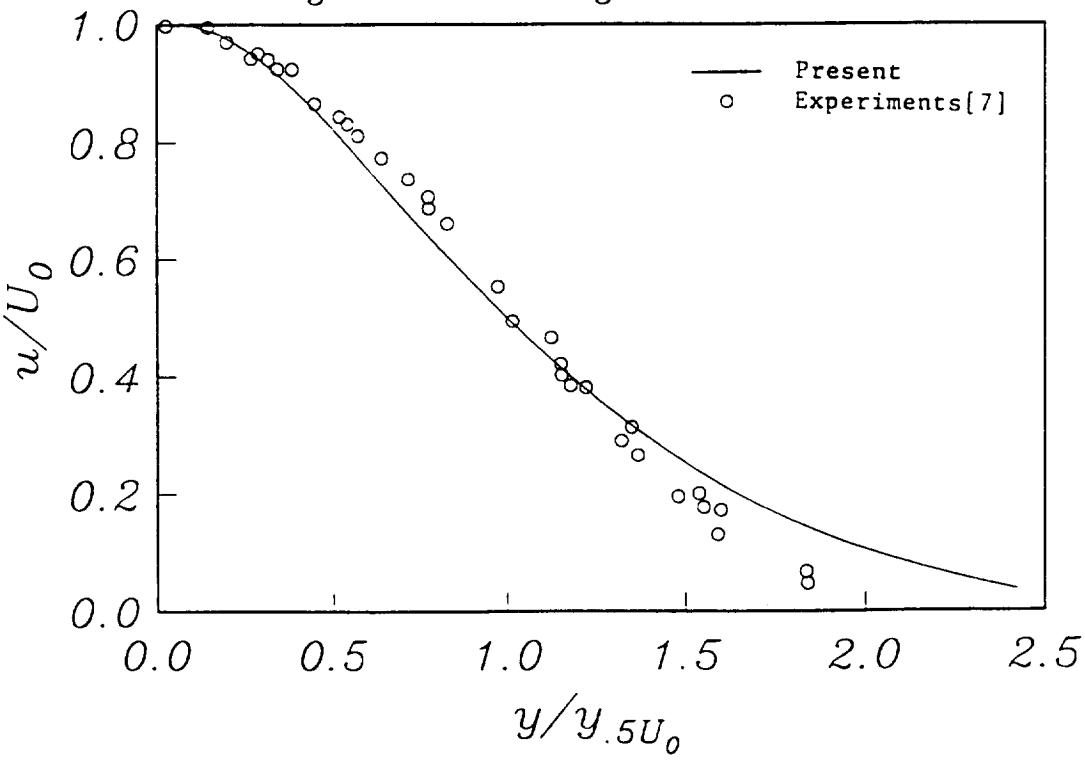


(U) The numerical solution for the ensemble averaged pdf's of the temperature: $y/y_{0.5} = 0.44$, where $y_{0.5}$ is the location where $T = 0.5T_0$. In order to interpret the data, the ensemble averaged pdfs are integrated to obtain the approximate continuous pdf: $P = P^*(\Delta T)/\Delta T$. The result of this integration is shown as vertical bars. The normal distribution is plotted as a dotted line for comparison.



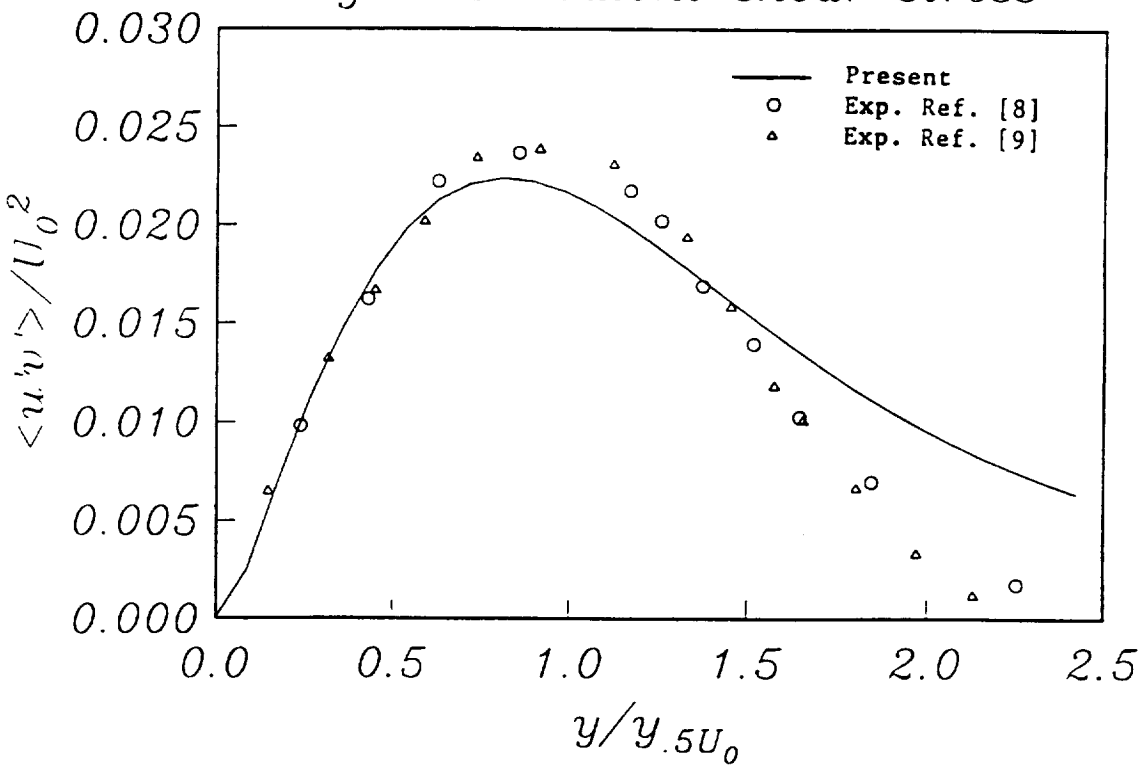
(U) The computed velocity profile is compared with experimental data from Foerthmann[7]. The good agreement between the numerical solution and experiments indicates that the parabolic flow solver employed in the present study is fairly accurate and can serve its purpose.

Fig.4 Velocity distribution



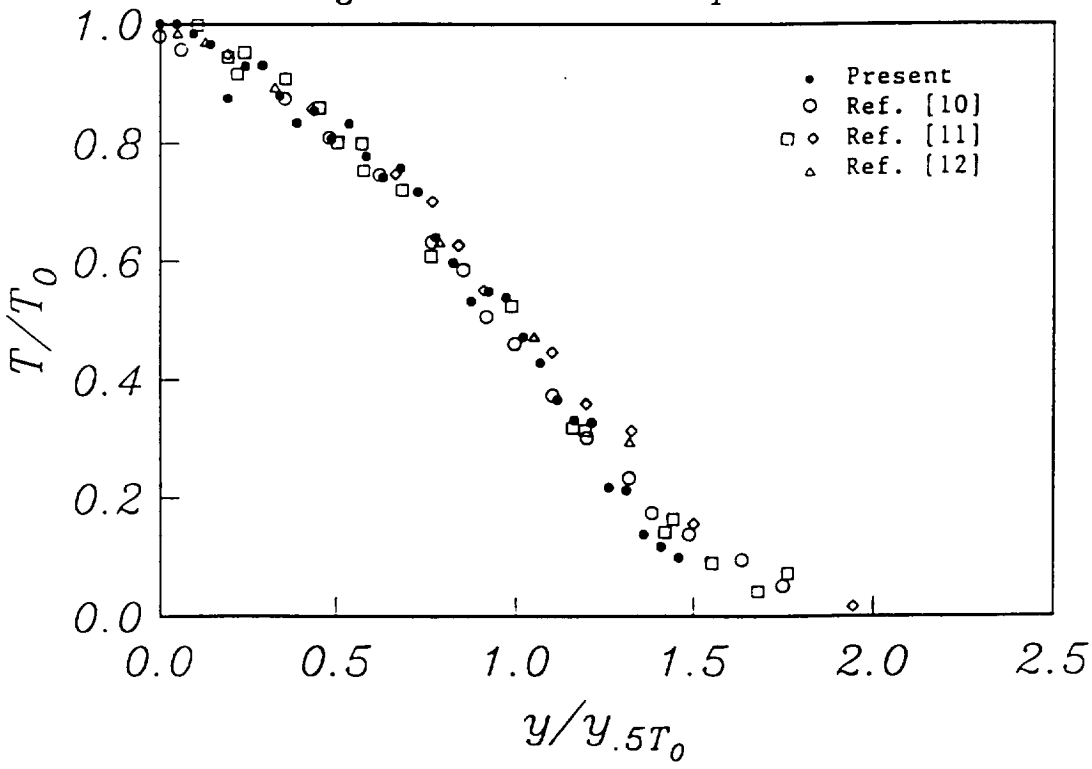
(U) As a calibration for the $k-\epsilon$ turbulence model, the turbulent shear stress from the present study is compared with measurements given by Brandbury[8], and by Gutmark and Wygnanski[9]. Except for a slight over prediction towards the edge of the jet, the numerical solution generally agrees well with the experimental data. This comparison is very crucial for pdf calculations because it is an indicator of the accuracy of the numerically predicted turbulent kinetic energy, k, and dissipation, ϵ, which are used to determine turbulent time scale, t, from $t = k/\epsilon$. An accurate prediction for k and ϵ is essential for the correct modeling of molecular mixing in the pdf calculation.

Fig.5 Turbulent shear stress



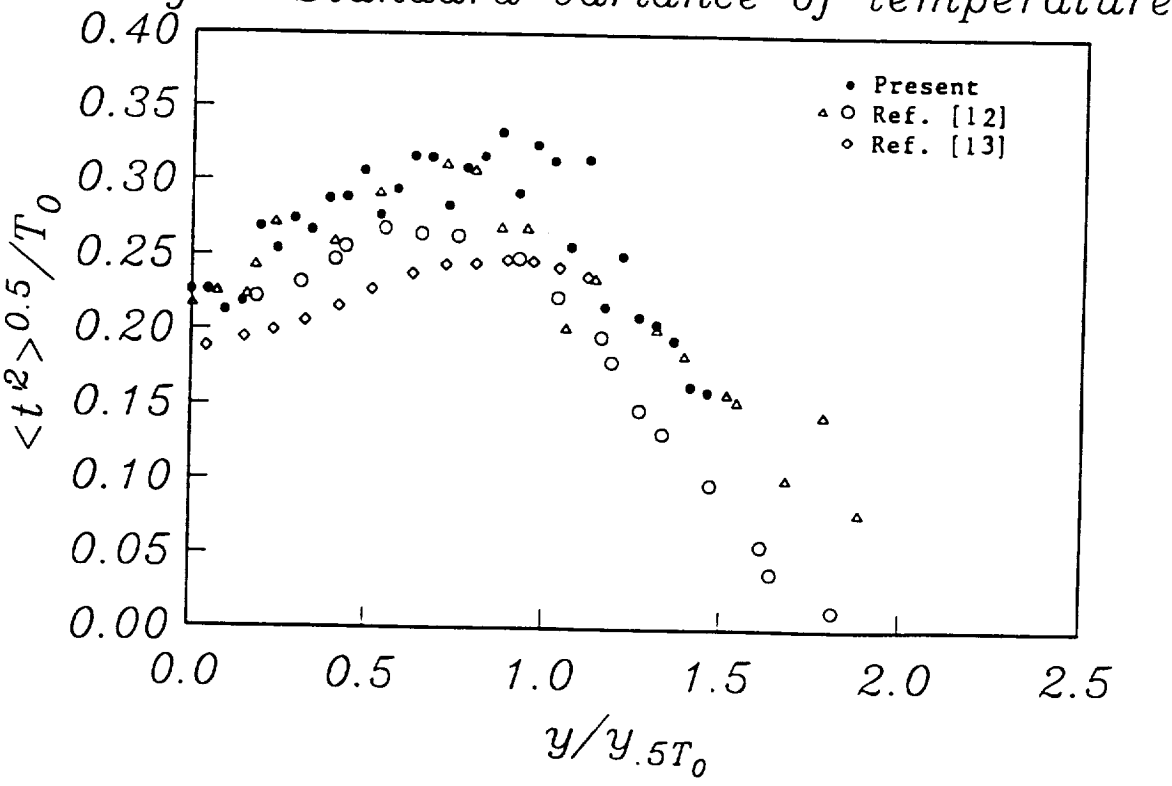
(U) The results for mean temperature from the Monte Carlo solution of the pdf equation for the temperature compared with experimental data from Ref. 10-12.

Fig.6 Mean temperature



(U) The standard variance of the temperature, or the temperature fluctuation, compared with experimental data from Ref. 12 and 13. Because of the limited number of sample points (N=100) used in the computation, the numerical results are scattered; however, these results agree very well with the experimental observations. Particularly important is the agreement between the predicted and the measured temperature fluctuations, for in case of finite rate chemistry calculations, the instantaneous temperature will be used in determining the reaction rate, and the correct prediction of the temperature distribution will ensure the accuracy in reaction rate calculations.

Fig. 7 Standard variance of temperature



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