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New Method for the Computation of Probability Density Functions in Turbulent Flows

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Introduction

It is now conventional to simulate the influences of the turbulence fluctuations in reacting flows with the aid of an assumed or calculated probability density function (pdf). In the case of diffusion flames, the thermodynamic state of the fluid is solely a function of the mixture fraction f (strictly true for negligible radiation transfer and equal diffusion coefficients for species and enthalpy). Knowledge of the one-dimensional pdf, p(f), permits a complete description of the flame. Perfectly premixed flames are described by a single progress variable, the reactedness τ. The possible forms for p(f) are restricted by limited turbulence-modeling knowledge to those specified by their first and second moments.

There may be special engineering circumstances where otherwise apparently satisfactory assumptions for p(f), perhaps those associated with the strongly temperature-dependent NO kinetics, are less than sufficient. Also, for the general case of partially premixed combustion, knowledge of the two-dimensional joint probability p(f,τ) is necessary, for which there is no guiding experimental evidence. Some means of calculating mono- or multidimensional pdf's becomes attractive, and the usual procedure is to solve for the required pdf in its own modeled-transport equation (see Refs. 1-3). An additional advantage of this procedure is that the chemical kinetics source term is closed so that finite-rate kinetics are accommodated without approximation regardless of the complexity of the reaction scheme.

The disadvantage of this approach is that the dimensionality of the calculation increases as the dimensionality of the pdf, and for traditional finite-difference-solution techniques the computational burden increases more or less exponentially with dimensionality. Even recourse to a fast-kinetics method results, for the usual three-dimensional engineering flow, in a pdf transport equation of five dimensions: x_1, x_2, x_3, f, and τ. In an effort to alleviate the otherwise unacceptable computer load associated with multidimensional problems, Pope[4] has constructed a Monte Carlo simulation of the transport equation having the considerable advantage that the computer time increases only linearly with dimensionality, although the storage requirement is large. Experience in the field of thermal radiation, where Monte Carlo theory is widely employed, led us to surmise that a recent and very economical method for thermal radiation calculations[5] might also be applied to the solution of the pdf transport equation with similar advantages. This has indeed turned out to be true, and the application is the subject of this Note.

Transport Equation

Derivation of the transport equation for the probability distribution function is given by Janicka et al.,[3] among others. Testing of physical models is not the concern of this Note. We have rather arbitrarily chosen to use most of the modeling employed in Ref. 3. The resulting form of the equation [Eq. (28) of Ref. 3] is

$$-\bar{\rho}\frac{\partial \tilde{P}}{\partial t}+\frac{\partial}{\partial x_i}\frac{\mu_{\text{eff}}}{\sigma_p}\frac{\partial \tilde{P}}{\partial x_i}-\bar{\rho}\tilde{u}_i\frac{\partial \tilde{P}}{\partial x_i}-\bar{\rho}\frac{\Gamma_0}{\tau_f}\tilde{P}$$
$$=-\frac{\bar{\rho}\Gamma_0}{\tau_f}\left[\int_0^z \mathrm{d}z,\tilde{P}_f(z')\int_z^1 \mathrm{d}z''\,\tilde{P}_f(z'')\tilde{P}(z',z'',z)\right]$$
$$+\bar{\rho}\frac{\partial}{\partial z}\left(\frac{S_0(z)}{\rho(z)}\tilde{P}\right) \tag{1}$$

where μ_{eff}, σ_p, $\bar{\rho}$, Γ_0, S_0 are considered known, z is, in the present case, normalized temperature, and $\sim$ and $-$ designate Favre and conventionally averaged quantities. The turbulence time scale τ_f is made equal to $k/(2\epsilon)$.

The present method is, by way of example, applied to a steady-state nonreacting flow. Equation (1) may after some working be written to represent transport along any particular fixed direction as follows:

$$\frac{\mathrm{d}}{\mathrm{d}s}\frac{\mu_{\text{eff}}}{\sigma_p}\frac{\mathrm{d}\tilde{P}}{\mathrm{d}s}-\bar{\rho}\tilde{u}_s\frac{\mathrm{d}\tilde{P}}{\mathrm{d}s}-\frac{\bar{\rho}\Gamma_0}{3\tau_f}P=-\frac{\bar{\rho}\Gamma_0}{3\tau_f}S \tag{2}$$

where s is a small distance along the path of calculation, u_s is velocity in that direction, and S represents the appropriate part of the right-hand side of Eq. (1). Integrating Eq. (2) over the whole solid angle around any point Q in the solution field yields Eq. (1). There is no difficulty in generalizing the analysis to unsteady finite-chemistry flows.

Here a second-order partial differential equation that has no simple analytical solution has been converted to an ordinary differential equation in a fixed direction whose analytical solution is known. This conversion has major implications for the solution of equations of the flow type.

Solution of the New Transport Equation

Equation (2) can be simplified by defining the appropriate coefficients Γ, u, and E, yielding:

$$\frac{\mathrm{d}}{\mathrm{d}s}\Gamma\frac{\mathrm{d}\tilde{P}}{\mathrm{d}s}-u\frac{\mathrm{d}\tilde{P}}{\mathrm{d}s}+E\tilde{P}=ES \tag{3}$$

This equation describes the change in the pdf of a scalar along any given straight line. Let us consider a particular line in the direction of s. Given pdf, $\tilde{P}_n$, and its derivative in the same direction, $\mathrm{d}\tilde{P}_n/\mathrm{d}s$ at the nth point on the line, then $\tilde{P}_{n+1}$ and $\mathrm{d}\tilde{P}_{n+1}/\mathrm{d}s$ can be calculated at the $(n+1)$th point on the same line using the simple analytic recurrence relation described below.

The analytical integration between the nth and $(n+1)$th locations assumes S is constant between these two points. This is equivalent, for instance, to assuming that the source is constant within a cell in a finite-difference-solution procedure, the normal practice. The form of the recurrence formula depends on the value of the coefficients of Eq. (3), assuming Γ is never equal to zero.

i) If $u=0$ and $E=0$, then

$$\tilde{P}_{n+1}=\frac{\mathrm{d}\tilde{P}_n}{\mathrm{d}s}s+\tilde{P}_n \tag{4a}$$

ii) If $E=0$, then

$$\tilde{P}_{n+1}=\frac{\mathrm{d}\tilde{P}_n}{\mathrm{d}s}\frac{\Gamma}{u}\left(e^{(u/\Gamma)s}-1\right)+\tilde{P}_n \tag{4b}$$

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iii) Let us define $\lambda^2 = u^2 - 4E\Gamma$. If λ^2 is greater than zero, and also defining

$$K_1 = (u+\lambda)/2\Gamma \text{ and } K_2 = (u-\lambda)/2\Gamma$$

then

$$\tilde{P}_{n+1} = Ae^{K_1 s} + Be^{K_2 s} + S \tag{4c}$$

where

$$A = \frac{K_2(\tilde{P}_n - S) - (d\tilde{P}_n/ds)}{(K_2 - K_1)}$$

and

$$B = \frac{K_1(\tilde{P}_n - S) - (d\tilde{P}_n/ds)}{(K_1 - K_2)}$$

iv) If $\lambda^2 = 0$, define $K_1 = u/2\Gamma$, then

$$\tilde{P}_{n+1} = \left[\frac{d\tilde{P}_n}{ds} s + (1 - K_1 s)(\tilde{P}_n - S)\right] e^{K_1 s} + S \tag{4d}$$

v) If $\lambda^2 < 0$, define $K_1 = u/2\Gamma$, $K_2 = (\sqrt{-\lambda^2})/2\Gamma$, then

$$\tilde{P}_{n+1} = e^{K_1 s}\left\{\left[\frac{(d\tilde{P}_n/ds) - K_1(\tilde{P}_n - S)}{K_2}\right]\sin K_2 s + (\tilde{P}_n - S)\cos K_2 s\right\} + S \tag{4e}$$

Equation (2) is solved at any point Q by tracing back from Q along lines of arbitrarily chosen direction to locations where $\tilde{P}$ and $d\tilde{P}/ds$ are known. The solid angle about Q is

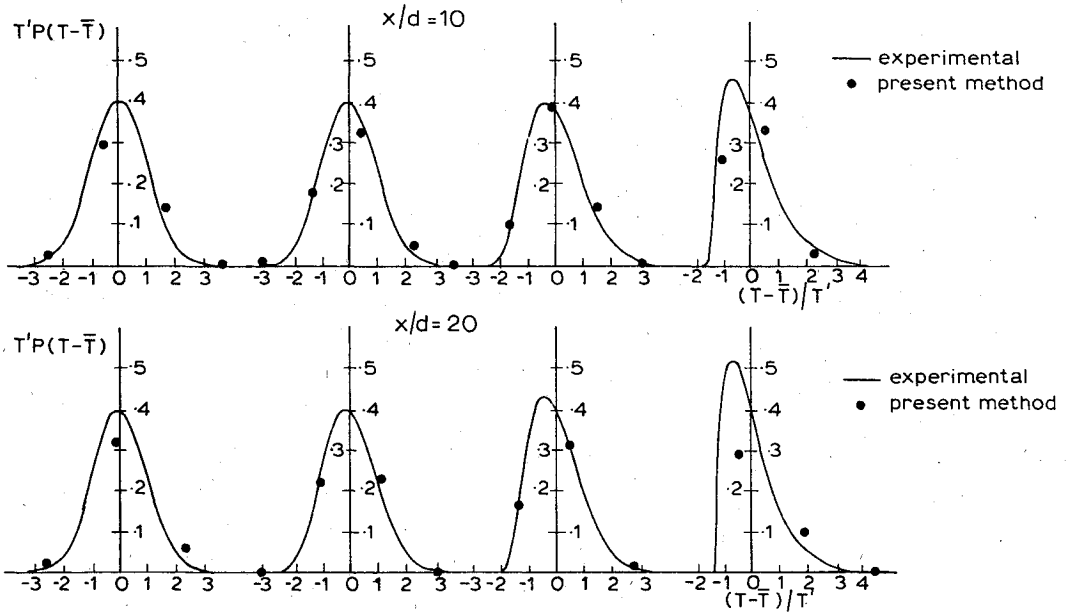

Fig. 1 Comparison of predicted (·) and experimental (—) pdf's along a radius $d \equiv$ pipe diameter. (Experimental pdf's from Ref. 6.)

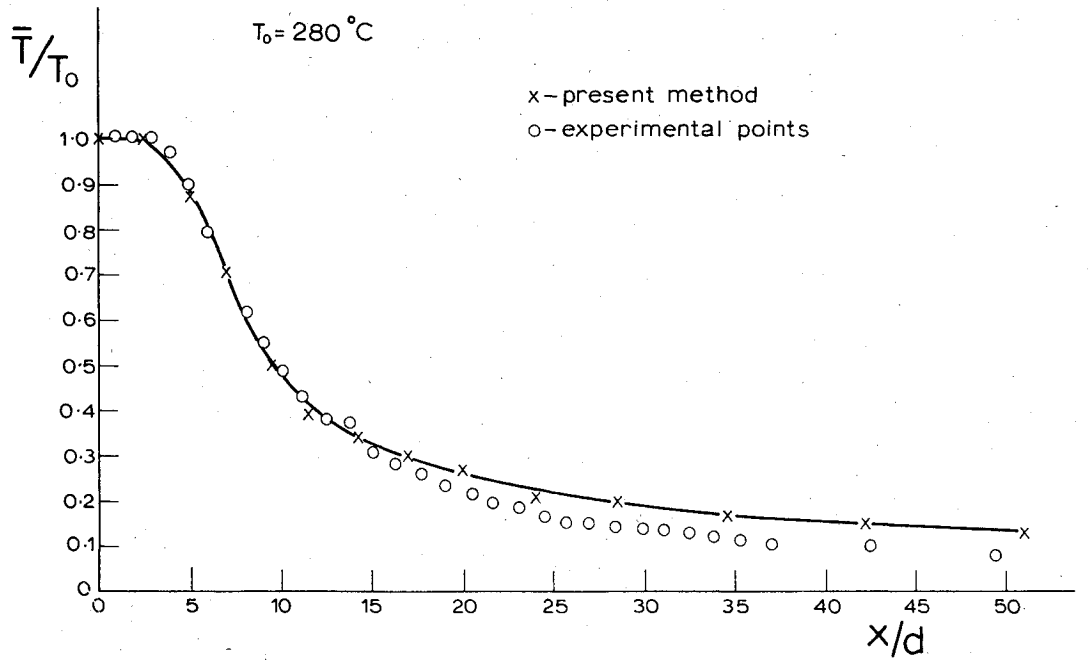

Fig. 2 Comparison of predicted and measured mean temperatures along jet axis. (Measured temperature from Ref. 6.)

considered to be discretized into subangles about these line directions. The solutions so obtained result in a set of $\tilde{P}$ at Q. The desired solution is that of Eq. (1), and it is obtained by integrating the sets of $\tilde{P}$ over their respective solid angles. Since each $\tilde{P}$ is considered to be constant over the subangle it represents, the integration amounts simply to an arithmetic weighting.

An Application of the Method

Temperature data, including pdf's, are reported in Ref. 6 for a fully turbulent jet having an inlet pipe Reynolds number of 5.04×10^4 and inlet temperature of 295°C. Field values of the mean flow quantities u_s, $\bar{\rho}$, μ_{eff}, k, and ϵ occurring in the pdf transport equation (2) were obtained from a standard (TEACH) parabolic prediction procedure incorporating the $k \sim \epsilon$ turbulence model. The recurrence relations (4) for $\tilde{P}$ are superimposed on this background. No attempt has been made to optimize the results by adjusting model parameters.

The method applies to the heated jet without restrictions. Since, however, only the upstream conditions significantly affect the downstream nodes, only the upstream hemisphere of the solid angle is included. Also, such variables as u_s, μ_{eff}, and ρ in the parabolic flow program are stored only for the current and the previous steps. The appropriate recurrence relation (4) is applied only between the adjacent preceding, or upstream, and current, or downstream, stations. Finally, since the influences from very far nodes have small effect on the solution, considerable computational time may be saved by suitably terminating the line calculation.

In order to calculate the temperature pdf, its range is subdivided into a finite number of discretizations. The relations (4) are applied to each discretization. This yields a pdf at the point Q for each line direction. The full solution is obtained by summing for each discretization the individual contributions for each direction. The method retains the properties of the pdf as the calculations proceed, so, for example, the integrated probability is always unity.

In Fig. 1 the mean values of the predicted temperature pdf's are compared with the mean temperature data along the axis of the jet. Such a comparison represents a particularly stringent test of a prediction procedure since the centerline decay of temperature is sensitive to the rate of jet spread, the good prediction of which is especially difficult to secure over the whole of the downstream region. A discrepancy emerges far downstream which is not too significant. Since the relation between temperature and a mixing parameter is linear, Fig. 1 may be interpreted as a measure of the validity of the prediction of the various mean flow quantities on which the pdf predictions are based.

Figure 2 shows a comparison between the predicted and measured pdf's along radii at two axial stations: $x/d = 10$ and 20. The predicted values are rather few. The whole of the temperature range between jet inlet and surroundings was subdivided into 10 increments whereas downstream the temperature activity does not span the whole of this range. There would be no difficulty in procuring more predicted values in the downstream region by a finer and not necessarily uniform discretization there. Bearing in mind that no modeling adjustments have been made, agreement is remarkably good. One can note that the time scale τ_f is that of velocity whereas the scalar time scale may be significantly different; it would be interesting to test the sensitivity of the results to this quantity.

Concluding Remarks

The technique is easily adapted to individual problems regardless of their geometrical complexity. We find the economy of the technique particularly appealing since, apart from the assumption of constant coefficients over δs, the recurrence relation is exact, so the true solution is more accurately approximated than for finite differencing relying on a conventional Taylor series quadratic truncation. As mentioned, the present line solutions may be terminated in regions of small interest, which is not possible with finite-difference techniques based on matrix inversion. Its memory requirement is especially small: only P and grad P are stored and, in the case of a parabolic flow, only at the previous station. In addition, there are no inherent statistical errors associated with the machine random number generation, as is the case with Monte Carlo methods.

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