ADVANCES IN PDF METHODS FOR TURBULENT COMBUSTION

Stephen B. Pope
Mechanical & Aerospace Engineering
Cornell University, Ithaca, NY 14853
pope@mae.cornell.edu

ABSTRACT

This paper reviews the recent advances made by the author's research group in applying PDF methods to turbulent combustion. Calculations of nonpremixed turbulent jet flames and their comparison to experimental data clearly demonstrate the ability of PDF methods accurately to describe finite-rate turbulence-chemistry interactions including local extinction and re-ignition. Numerical methods and algorithms are crucial to the application of PDF methods to practical combustion problems. The stand-alone particle mesh method used in the code PDF2DV, though convergent, has been found to be inefficient because of a substantial bias error. Consistent hybrid algorithms have been developed which are both accurate and efficient. The method of *in situ* adaptive tabulation (ISAT) is essential to the computationally efficient implementation of combustion chemistry. Advances to the original algorithm have recently been made. PDF methods are being developed to serve as subgrid scale models in LES of turbulent reactive flows.

INTRODUCTION

The difficulty of predicting the behavior of constant-density inert flows is compounded manyfold in the case of turbulent combustion. A realistic description of hydrocarbon combustion chemistry requires consideration of approximately 20 species, whose reaction rates are nonlinear functions of temperature and of the species concentrations. The combination of these nonlinearities with the large property fluctuations associated with turbulence lead to the turbulence-chemistry closure problem. Compared to moment closures (either at the RANS or LES levels), PDF methods essentially overcome this closure problem.

Over the past 10 years at Cornell, our focus has been on the modelled transport equation for the joint probability density function (PDF) of velocity, turbulence frequency and composition (species mass fractions and enthalphy). Background on PDF methods is provided by Pope (1985, 2000) while the turbulence modelling involved is described by Van Slooten, Jayesh & Pope (1998) and by Subramaniam & Pope (1998).

The modelled PDF transport equation is solved by a particle/mesh method. Within each grid cell, the joint PDF is represented by an ensemble of N_{pc} particles, each particle having a given mass, velocity, turbulence frequency and thermochemical composition. The solution evolves by these particle properties evolving in time. For steady-state problems the particles continuously evolve, but Eulerian statistics deduced from them attain a statistically-stationary state. Considerable effort has been expended on developing more accurate and efficient particle methods to facilitate the application of PDF methods to practical flows.

In the subsequent sections of this paper we review: recent applications of PDF methods to nonpremixed piloted jet flames; the development and evaluation of different particle methods; the ISAT algorithm for implementing combustion chemistry; and the combination of PDF and LES methodologies.

NONPREMIXED PILOTED JET FLAMES

The experimental data of Barlow & Frank (1998) provide—by design—an excellent test of turbulent combustion models. A sequence of flames A–F is studied, in which the jet velocity is increased from a laminar flame (A) to a fully turbulent flame with little local extinction (D) to a flame on the verge of blow-off (F). Scatter plots and conditional statistics obtained from spatially and temporally resolved laser diagnostics clearly show the phenomenon of local extinction and subsequent reignition.

PDF calculation of the Barlow & Frank flames are reported by Xu & Pope (1999) and by Tang, Xu & Pope (2000). In the first paper a 16-species mechanism for methane (without nitrogen chemistry) is used; in the second paper 19 species are used to include NO for-

mation (Sung, Law & Chen 1998). The calculated and measured scatter plots appear to be in excellent agreement. To quantify the comparison, a burning index (BI) is defined to characterize the level of extinction (BI = 1 corresponding to complete combustion; BI = 0 to complete extinction). The PDF calculations are able to represent quite accurately the experimentally observed dependencies of BI on the jet velocity and on axial distance.

The later calculations of Tang et al. (2000) include radiative heat loss and the calculation of *NO*. It is found—in retrospect not surprisingly—that the calculations of flame F (which is close to blow-off) are very sensitive to the specified temperature of the pilot stream (which is not known precisely in the experiment).

PARTICLE-MESH METHODS

Over the last 5 years we have moved from a stand-alone particle-mesh method (PDF2DV, Pope 1994), to a consistent hybrid method (Muradoglu et al. 2000).

In a comprehensive numerical study, Xu & Pope (1999) showed that PDF2DV is second-order accurate in space, and that the solution converges as the number of particles per cell (N_{pc}) tends to infinity. But it was also found that PDF2DV has a substantial bias—that is, a deterministic numerical error that decays as N_{pc}^{-1}. As a consequence, a large number of particles ($N_{pc} \approx 2,000$) is needed to obtain accurate results (i.e., less than 5% numerical error in all variables examined). To alleviate this problem, Xu & Pope (1999) developed an extended Richardson extrapolation technique in which two calculations are performed on different grids and with (an appropriately chosen) different value of N_{pc}. From the two solutions, an extrapolated solution is obtained which is free of leading-order truncation error and bias.

In an attempt to eliminate or substantically reduce the bias experienced by stand-alone particle methods, several hybrid methods have been developed and evaluated (Jenny et al. 2001 a,b, Muradoglu et al. 1999, 2000). In a hybrid method, equations are solved for mean fields (e.g., mean velocity and pressure) by a conventional finite-volume technique, in addition to the PDF equations being solved by a particle method. This approach results in duplicate fields and redundant information, and consequently can lead to inconsistencies. Indeed the early PDF calculations of Pope & Correa (1988) are based on an inconsistent hybrid method (the code pdf2ds).

Consistency is considered at the level of the differential equations to be solved and also at the level of the numerical solutions. Consistency at the level of the differential equations is simply and automatically achieved by deriving the mean field equations from the modelled joint PDF equation. Muradoglu et al. (2000) identify various consistency conditions at the numerical level and show that only three of these are independent. These conditions can be taken to be the equality of the mean velocity and energy fields, and the consistency of the particle mass density. For each of these conditions a corresponding correction algorithm has been developed to enforce consistency at the numerical level.

The consistent hybrid algorithms have, as hoped, proved to be essentially bias-free. As a consequence, for the same level of accuracy compared to PDF2DV, a factor of 100 fewer particles are required, leading to a comparable increase in computational efficiency. Jenny et al. (2001b) compare the performance of PDF2DV with two hybrid algorithms. Reassuringly, the three codes converge to the same result, with the hybrid algorithms requiring far fewer particles for given accuracy.

IN SITU ADAPTIVE TABULATION (ISAT)

An important advance in the past five years has been the development of augmented reduced mechanisms (ARM) for methane combustion (Sung, Law, and Chen 1998). These mechanisms account for of order 20 species, and are derived from comprehensive 50 species mechanisms. These ARMs have been found to be accurate over a very broad range of conditions—in marked contrast to simpler, earlier, four-step mechanisms.

When the PDF particle method is applied to a turbulent combustion problem, on each time step each particle's composition is advanced for a small time interval Δt to account for the effects of reaction. In a typical computation there are of order 10^9 particle steps (e.g. 60 $\times$ 60 cells, $N_{pc} = 100$ particles per cell, 3000 time steps). The straightforward approach is direct integration (DI): that is, the set of 20 stiff ODEs for the evolution of the thermochemical composition given by the ARMs is integrated numerically. To do so once is not difficult, thanks to the development of accurate and reliable stiff ODE solvers: but to do so 10^9 times is prohibitive.

It is preferable instead to tabulate the results of the ODE integration and to advance the particle composition by a table-look-up.

This approach has long been standard with simple chemistry descriptions for which a table with 1,2, or 3 dimensions is readily generated in a pre-processing phase. However, it is highly non-trivial in a 20-dimensional composition space; and, indeed, at first sight it may seem impossible. But it is now understood that the compositions that occur in combustion do not fill the 20-dimensional composition space, but instead lie close to low-dimensional manifolds (Maas & Pope 1992a,b). An algorithm has been devised (Pope 1997) which constructs a table *in situ* as the PDF calculation is being performed. In this way, only the accessed region of the composition space is tabulated. The resulting ISAT algorithm has effective error control, so that interpolation error is (with high probability) less than a specified tolerance.

In simple test problems ISAT is faster than DI by a factor of 1,000. For a variety of reasons, this factor may be reduced to about 40 in a typical PDF calculation. A new version of the ISAT code (ISAT-CK) has recently been developed with enhanced capabilities and performance compared to the original code.

PDF METHODOLOGIES IN LES

LES has long been touted as the methodology most suited for addressing turbulent flow problems in engineering and other applications. The author's view is that a full range of approaches—from mixing length to LES—is useful (Pope 2000), and, further, that LES is many years from fulfilling its promise.

In turbulent combustion, LES has the natural advantage over RANS approaches of directly representing the large-scale unsteady motions that often occur in combustion devices. It should be fully appreciated, however, that LES suffers the same closure problem as RANS, with respect to the turbulence-chemistry interactions (Pope 1990). As observed by Pope (1990), the PDF methodology can be used in LES to avoid the turbulence-chemistry closure problem. Specifically, the filter-density function (FDF) can be defined which has similar properties to the PDF. The evolution equation for the FDF was subsequently derived by Gao & O'Brien (1993).

The LES/FDF methodology has been implemented by Colucci et al. (1998), Jaberi et al. (1999), and Gicquel et al. (2001). The first two of these works uses the (equivalent of the) composition PDF method, while the third uses the velocity-composition method. This approach is, of course, computationally intensive. Further, several aspects of the new consistent hybrid algorithms depend on the statistical stationarity of the solution and hence are not applicable to LES/FDF.

CONCLUSIONS

PDF methods for turbulent combustion have reached a level of maturity. The physical models are well-developed and understood, even if their performance is not always as good as desired—as is the case with all turbulence models. Efficient numerical algorithms have been developed, both the hybrid particle method and ISAT. Comparisons with experimental data have clearly demonstrated the capability of PDF methods to account accurately for turbulence-chemistry interactions. The major impediment to the wider use of PDF methods in engineering applications is the lack of availability of a suitable code. This impediment is likely soon to be removed, as PDF methods become available in commercial CFD codes.

The standard PDF and LES approaches have different advantages and limitations. LES has the advantage of directly representing large-scale unsteady motions, and hence may be the preferred approach to problems such as combustion instabilities. PDF methods have the advantage of accounting for turbulence-combustion interactions, and enable the use of realistic chemistry. It is likely that in this decade, these two approaches will be used when unsteady effects and chemistry, respectively, are the most important feature. In the longer term, when the computational power is available, the advantages of both approaches can be exploited through LES/FDF. History shows that developing numerical algorithms is often the rate-limiting process: hence it is timely to further develop the LES/FDF methodology.

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