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ADP023647

TITLE: PDF Modeling of Turbulent Combustion

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TITLE: Army Research Office and Air Force Office of Scientific Research Contractors' Meeting in Chemical Propulsion Held in Arlington, Virginia on June 12-14, 2006

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PDF MODELING OF TURBULENT COMBUSTION

AFOSR Grant FA-9550-06-1-0048

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SUMMARY

In both space and aircraft applications, the design of combustors in propulsion systems remains a significant technical challenge. Given the cost, difficulty and time consumed in experimental testing, it is well recognized that computer modeling is essential to exploring different design concepts, and to reducing the cost and time of the design cycle. While many phenomena may be involved – sprays, radiation, combustion dynamics, etc. – a central problem is that of modeling turbulent-chemistry interactions in turbulent combustion. The PDF approach to turbulent combustion has the advantages of fully representing the turbulent fluctuations of species and temperature, and of allowing realistic combustion chemistry to be implemented (e.g., of order 50 species). This methodology is also being applied in conjunction with large-eddy simulations, in which case it is referred to as LES/FDF. The overall objective of the proposed work is to advance and extend the PDF and LES/FDF approaches to modeling turbulent combustion in flows of relevance to aerospace propulsion systems. Currently, PDF methods are being applied to flames in vitiated co-flows, both lifted methane non-premixed flames and also attached piloted premixed flames. In future work, the LES/FDF approach will be applied to piloted jet flames and to bluff-body jet flames. This will enable a three-way comparison between experimental data, the LES/FDF calculations, and previous PDF calculations. In all of these calculations, realistic and reliable combustion chemistry is used (e.g., involving of order 20-50 species) so that turbulence-chemistry interactions such as local extinction and re-ignition can be investigated. Collaboration with the University of Pittsburgh continues and has resulted in one of the first LES/PDF calculations of a turbulent flame (Sheikhi *et al.* 2005).

PDF CALCULATIONS OF PILOTED JET FLAMES

The Barlow & Frank (1998) piloted jet flames are well recognized as providing an excellent test of turbulent combustion models, in particular of their ability to describe local extinction and re-ignition. There is a sequence of flames *A–F*, with *D*, *E*, and *F* being fully turbulent, with increasing amounts of local extinction. While there are many successful modeling studies of flame *D* – which has little local extinction – there are far fewer of the more challenging flames *E* and *F*.

PDF methods have previously been successfully applied to these flames by Xu & Pope (2000), Tang *et al.* (2000), and Lindstedt *et al.* (2000). Since the Cornell and Imperial College groups use different mixing models and different chemical mechanisms, questions arise as to the dependence and sensitivity of the calculations to these ingredients. Some progress has been made in understanding the relative behavior of the different mixing models (see, e.g., Ren &

Pope 2004). We have now concluded a series of PDF calculations addressing these issues. Cao & Pope (2005) describe joint PDF calculations of these flames using 7 different chemical mechanisms for methane, ranging from a 5-step reduced mechanism, to the 53-species GRI 3.0 mechanism. The results show that the GRI mechanisms (and the augmented reduced mechanisms based on them) are capable of accurately representing the observed local extinction and re-ignition. In contrast, C_1 skeletal mechanisms and 5-step reduced mechanisms prove to be inaccurate.

This work has been followed up by a study (Cao *et al.* 2006) of the influence of the turbulent mixing models used in the PDF model calculations. The principal finding is that (with a different value of the mixing-model constant) all three commonly used models (IEM, MC and EMST) are capable of yielding the observed level of local extinction. But only the EMST model produces, simultaneously, the observed level of mixture fraction fluctuations.

PDF CALCULATIONS OF LIFTED TURBULENT FLAMES

In laboratory experiments on turbulent flames, for obvious reasons, air at atmospheric conditions is generally used as the oxidant. In practical applications, however, the re-circulating flows used for flame stabilization generally lead to some mixing between the air stream and hot combustion products. And in thrust augmentors the oxidant stream is simply the lean combustion products from the turbine.

Motivated by these observations, a series of experiments has been performed (at Berkeley, Sandia, and Sydney) on various jet flames in vitiated co-flows. Previously we have performed two PDF studies of the lifted hydrogen flames studied experimentally by Cabra *et al.* (2002). These two studies are based on the composition PDF method incorporated in Fluent (Masri *et al.* 2004), and on the velocity-frequency-composition joint PDF method (Cao, Pope & Masri 2005). In both cases, detailed 9-species mechanisms for hydrogen are used.

We are currently investigating the lifted methane flames studied by Cabra *et al.* (2002, 2005). The calculations are based on the joint PDF method used previously, with the modified Curl mixing model and the ARM1 mechanism. Some preliminary results are given in Fig. 1. As may be seen, for the most part there is good agreement between the calculations and the measurements, but there are some discrepancies for CO and OH.

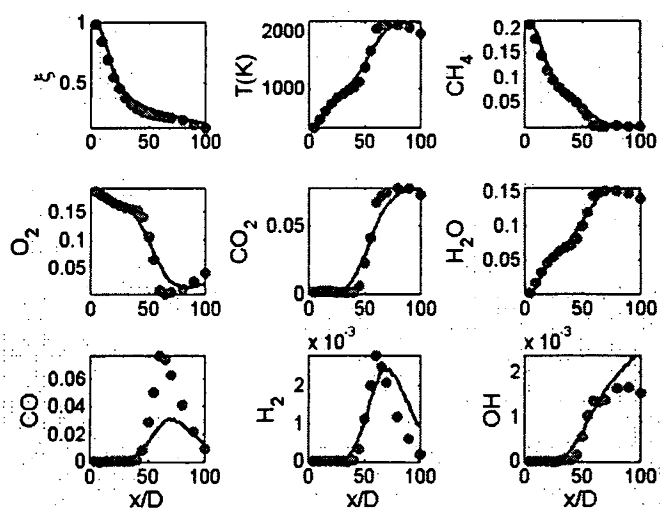

Fig. 1. Centerline profiles of mean mixture fraction, temperature and mass fractions of CH_4, O_2, CO_2, H_2O, CO, H_2 and OH. Symbols: Measurement by Cabra et al. 2005; Lines: Joint PDF calculations.

The PDF method calculations presented above demonstrate current capabilities, e.g., using a mechanism with of order 50 species. Such calculations are possible because of the ISAT algorithm (Pope 1997) and the availability of parallel computers. As we work towards combining PDF methods with large eddy simulation (LES), larger parallel clusters are needed, and the efficient parallel implementation of ISAT becomes critical.

If there are P processors, then the load associated with solving the LES equations is well balanced if the solution domain is partitioned into P sub-domains, each containing approximately the same number of cells. Further, with such a decomposition, the computational particles used in the PDF algorithm are approximately equally distributed between the processors. Hence there is good load balancing of particle tracking and of mixing. However, the load associated with reaction (i.e., incrementing the particle compositions due to reaction over the time step) which can dominate the CPU time can be poorly balanced. For example, the particles on one processor may be inert (e.g., cold air) and hence require negligible time to evaluate their reaction; whereas the particles on another processor may be highly reactive. Even using ISAT, reactive particles take much longer to treat, especially if retrieving from a full table is not possible, and hence a direct integration of the stiff ODEs is required.

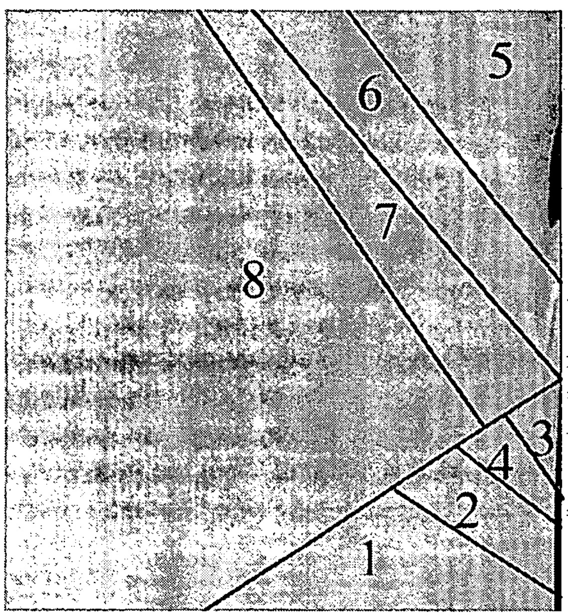

Fig. 2 Contour plot of mean temperature in PDF calculations of a lifted hydrogen jet flame, showing the sub-domains used in the Fluent parallel computation.

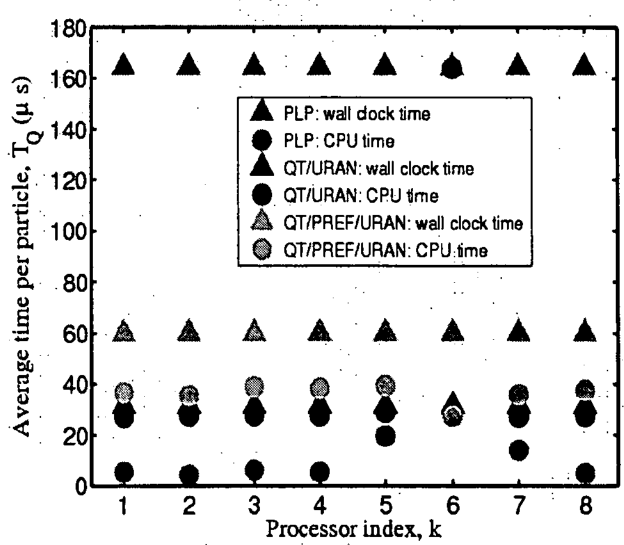

Fig. 3 Average wall clock and CPU times (per particle per reaction fractional step) for parallel Fluent computations of the lifted hydrogen flame, with different parallel ISAT strategies.

Following the preliminary work of Lu *et al.* (2005), we are continuing to develop and evaluate parallel strategies for implementing ISAT. One of the test problems considered is the composition PDF method in Fluent applied to the lifted hydrogen jet flame described above. Figure 2 shows the solution domain and its decomposition into the eight sub-domains used in the parallel computation (using 8 processors). Figure 3 shows the CPU and wall-clock times per particle step required by three different parallel strategies. The first is PLP (purely local processing) in which no message passing is performed, but each processor invokes ISAT independently for all of the particles in its sub-domain. As may be seen from the CPU times, there is considerable load imbalance with processor 6 requiring significantly more time. Note that the corresponding sub-domain is the base of the flame, which involves the most challenging ignition chemistry. The two (non-trivial) parallel strategies lead to speed-ups (relative to PLP) of about 2.5 and 5.

PUBLICATIONS

The following papers based on AFOSR sponsored research have been published or written in 2005-2006.

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