Panel discussion on computational combustion

By J. C. Hill[1]

A moderated panel discussion was held to gather opinions on the status of computational methods for turbulent combustion and to assess the role and usefulness of direct numerical simulations in fundamental studies of turbulent combustion and in the development of engineering predictive models. Panelists were F. A. Williams, S. B. Pope, and T. Poinsot. It is clear that computational models are in need of considerable work for combusting flows and that DNS can be useful in their development, in which canonical or simple problems are computed fully to validate a model or answer questions about the pertinent physics of the problem.

1. Introduction

An increasing portion of the research projects at the first four CTR summer programs deals with reacting flows –two of 30 in 1987, one of 23 in 1988, five of 25 in 1990, and six of 23 in 1992 (Moin *et al.* 1987, 1988, 1990, 1992). Several of the studies involve direct numerical simulations of 2-D and 3-D reacting flows, some with Arrhenius kinetics and others for isothermal systems, some with volume generation from heat release (compressible codes) and others for isochoric motions, some with simple reaction kinetics and others for systems with complex chemistry. Most of the studies are motivated by questions dealing with turbulent combustion, although some do not deal with the combustion problem *per se* but with simpler problems in order to answer specific questions about reacting flows.

In support of these studies, a panel discussion was held to review the status of computational models for turbulent combustion. (See Table 1 for an outline of available types of computer models, noting those for which production codes are available.[2]) A particular focus of the panel was to determine to what extent direct simulations are useful in support of these models or for investigating the fundamental physics of these flows. Indeed, there is a variety of degrees of refinement for DNS of turbulent combustion (constant/variable density, infinitely fast/finite rate chemistry, single step/complex chemistry). Due to resolutions requirements, the more elaborate the approach is, the more restricted the simulations are in terms

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2 Table 1 was prepared by D. C. Haworth with the assistance of the following members of the reacting flows research group: M. Baum, J. H. Chen, R. O. Fox, F. Gao, J. C. Hill, S. Mahalingam, T. Poinsot, I. K. Puri, D. Reuss, A. Trouvé, and L. Vervisch. The designation 'production code' indicates that computer models of that type are in common use by the gas turbine industry, IC engine companies, and parts of the chemical and petroleum processing industries in the opinions of the above group.

of Reynolds and Damköhler numbers. So it is useful to ask whether the best compromise might be found and, in particular, whether including more physics in the simulations does not result in tractable problems with characteristics far from the range of Reynolds and Damköhler numbers of interest. Consequently, it was felt desirable to step back and reflect on the situation.

The panel, moderated by W. C. Reynolds, consisted of the following members: F. A. Williams (University of California at San Diego), S. B. Pope (Cornell University), and T. Poinsot (CNRS, Institut de Mécanique des Fluides, Toulouse). The panelists delivered brief position statements (summarized in Section 2) and then responded to general questions in the discussion period (summarized in Section 3).

Table 1. Types of turbulent combustion models.[a] Listed in increasing order of complexity. "Production" codes are in use for models marked with an asterisk*.

	Turbulence Models	**Combustion Models**		
		Premixed	Diffusion	Premixed/diffusion
One-point, time- or ensemble-average	ℓ	Arrhenius*	Equilibrium*	
	k-ϵ*	EBU*	EBU*	
	ASM	EBU/Arrhenius*		EBU/Arrhenius*
	RSM	Simplified pdf	Simplified pdf*	
	pdf	Flamelet*	Flamelet*	Flamelet*
		Full pdf	Full pdf	Full pdf
Spatial filter	LES	Arrhenius	Equilibrium	
	RVM	G-equation	Arrhenius	

[a] Notations: ℓ denotes algebraic length models, ASM = algebraic stress model, RSM = Reynolds stress model, EBU = eddy breakup model, LES = large eddy simulation (with subgrid model), RVM = random vortex methods, Simplified pdf = assumed pdf methods, Equilibrium = fast chemistry assumption. Arrhenius models are usually based on mean concentrations and neglect turbulent fluctuations. There are various versions of EBU and flamelet models. The last column refers to situations such as in IC engines where flames are partially premixed and where both types of flames exist.

2. Position statements of the panelists

This section presents the basic ideas contained in the position statements of the panelists, as interpreted by J. C. Hill.

2.1 Models for computing turbulent combusting flows

(F. A. Williams, University of California at San Diego)

To provide some framework for discussion, F. A. Williams presented the following classification of the wide variety of computational models available for turbulent combusting flows (Liñán and Williams 1993): (1) 0–dimensional models (no turbulence), (2) moment methods including algebraic closures, k-ϵ(-g) models (KIVA, SPEED, FIRE, etc.), full second order models, (3) presumed pdf approximations using moments including BML and G-equation for premixed flames and mixture fraction for diffusion flames, (4) pdf evolution methods including C/D and LMSE closures, (5) extended perturbation methods including RNG and moment modeling of the G-equation, fractals, etc., (6) field methods not based on the conservation equations (age theories in CSTR's for example), and (7) DNS. There are a number of models in (1)–(6) that have resulted in production codes (*cf* Table 1), which have met with varying degrees of success; however, in category (7), only LES is possible for any practical problem, but it does not yet exist for combustion.

One of the overriding factors in selecting a model is the range of Da and Re in the problem at hand (See Fig. 2 in Williams 1985, which classifies the regimes). Other parameters are less important. Most models are for low to moderate Re_L, and (7) is currently only possible at low Re_L. No models seem to apply in the broken flamelet regime (high Re_L, moderate Da). To illustrate the difficulty of validating a model, experimental (laboratory) data for turbulent flame speed can vary over nearly an order of magnitude, and this is reflected by the more than half dozen commonly used expressions for the turbulent burning velocity S_t. Some theoretical estimates of S_t are clearly incorrect, and perhaps DNS can be of help, although extrapolation to high Re_L will be difficult.

2.2 Role of numerical simulation in the study of turbulent combustion

(S. B. Pope, Cornell University)

S. B. Pope makes the point that DNS of turbulent combustion cannot be done in the engineering context. For example, for a simple hydrocarbon–air reaction with 50 chemical species and 200 reactions with time scales differing by as much as a factor of 10^{10}, variable temperature and physical properties, and with the complex geometry of the combustor, DNS is not practicable with computer technology available now or in the near future. The way to proceed, however, is to use DNS to study phenomena in isolation by simplifying the problem until tractable, taking care to preserve the desired physics, and then using the results to develop statistical models which *can* be applied to practical problems, *i.e.* apply DNS to a model problem that contains an essence of the desired problem and which contains sufficient physics for the results to be useful (Pope 1990).

Examples were shown from S. B. Pope's own studies of the use of DNS in constant density, forced isotropic turbulence. These include the evaluation of the Reynolds number dependence of Lagrangian statistics of the velocity and acceleration fields

for a stochastic model suitable for engineering purposes (Yeung & Pope 1989), the evaluation of pdf's of mixture fraction (inert scalar field) in order to parameterize a mapping closure of mixing (Eswaran & Pope 1988, Pope 1991), and studies of the motion and curvature of material surfaces and stoichiometric surfaces (Pope *et al.* 1989, Yeung *et al.* 1990, Girimaji & Pope 1992) to determine characteristics needed for flamelet models; in the latter studies it was shown that curvatures become unbounded and that cusps form in finite times.

In summary, statistical models can be applied to practical problems and DNS cannot, but models applied to simple problems accessible to DNS are useful for testing their foundations. However, one needs to be careful of extrapolating Re- and Da- dependence.

2.3 Direct numerical simulations: one of the tools to study turbulent combustion

(T. Poinsot, CNRS, Institut de Mécanique des Fluides de Toulouse)

T. Poinsot presented several examples of the use of DNS to study turbulent premixed combustion. Applied to the flamelet approach, there is a three-fold computational problem: (1) the validity of the flamelet assumption has to be tested, then when this assumption is valid, it is necessary to compute (2) the flame surface density Σ and (3) the burning velocity or consumption rate per unit flame surface area, S_c. DNS computations have been made for 2-D and 3-D constant density and variable density flows, simple chemistry with Arrhenius kinetics and complex chemistry (including variable density in 2-D) (Rutland & Ferziger 1989, Cant *et al* 1990, Poinsot *et al.* 1991, Mahalingam 1989, Haworth & Poinsot 1992); in terms of the parameters u'/u_{flame} and l_t/L_{flame}, DNS with chemistry is approaching the range of these parameters of practical interest, at least for some simple problems (Haworth & Poinsot 1992). [Note: The latter point, particularly with regard to the IC modeling study mentioned in the next paragraph, was debated by the other panelists during the discussion period.]

Several features of the flamelet model have been examined by DNS; for example, it has been found that the flamelet structure is controlled not only by strain rate as assumed in the library approach, but also by flame curvature. In addition, strong effects of thermo-diffusive instabilities (Lewis number effects) on the flame surface evolution were found. Vortex–flame interaction studies have also been made to study quenching phenomena, and the results give further support to the flamelet model (Poinsot *et al.* 1991). DNS has been used in models of premixed flames (Meneveau & Poinsot 1991, Boudier *et al.* 1992, Bray & Cant 1991, Nicolleau *et al.* 1991) and has also inspired or followed new experiments on flame-vortex interactions, on the effect of Lewis number in turbulent jet flames, on flame speeds in curved flames, and on optical diagnostics (Roberts & Driscoll 1991, Poinsot *et al.* 1991, Wu *et al.* 1991). DNS has also been used to develop a new model implemented in KIVA to predict ignition in spark-ignited engines and to accurately describe such important effects as flame behavior at the wall, combustion efficiency, and equivalence ratio (Boudier *et al.* 1992).

In summary, it was shown that DNS is useful in building models of turbulent combusting flows and is also useful in improving our understanding of combustion. Future work is needed on the theory, especially for non-premixed flames, and for the DNS of complex chemistry in 2-D, simple chemistry in 3-D, and for more efficient parallel codes.

3. Discussion

In addition to some technical issues not reported here, the following principle points were raised in response to the presentations of the panelists:

- The following simplifications are common for DNS of reacting flows: (a) cold flows (constant T and ρ, 3-D Navier-Stokes, *i.e.,* the passive scalar problem) vs. flows with variable temperature; (b) incompressible (either constant T or with Arrhenius rate but with constant ρ) vs. compressible (Arrhenius kinetics with heat release; *i.e.,* couple hydrodynamics, energy, and reaction); (c) 2-D vs. 3-D simulations; (d) equilibrium vs. finite rate chemistry; simple (single-step) kinetics vs. complex chemistry, model vs. 'real' chemistry; (e) Fickian diffusion vs. multicomponent diffusion; (f) decaying vs. forced turbulence; (g) premixed or nonpremixed vs. partially mixed systems. It is apparent that such simplifications are necessary to make some problems tractable, and that the simplification made depends on the problem, with care taken that the essential physical properties are preserved. For example, if interested in mixing terms, isothermal simulations might be acceptable, if interested in complex chemistry with widely different reaction rate constants, 2-D simulations might prove sufficient, etc. In general, it was thought best to do the simpler simulations first (*e.g.,* 2-D without full chemistry) and then add complications, but within the context of a model or the physics being examined. Care must be taken with the simplifications, however; for example, the reverse energy cascade in 2-D may have some unexpected influence on flame surface density.
- A good problem to attack by DNS would be to do the fluid mechanics for the broken-flamelet regime in the case of non-premixed combustion. Also, it was clear from the discussion that there is no universal agreement on the mechanism of flamelet extinction.
- The next generation of machines (T-flop) may be able to shift the focus in DNS away from the archetypal simple problems to more practical problems, but as suggested above, doing the simpler problems first increases understanding.
- The prospects for LES and SGM in a reacting environment are not very good because of domination by small scales at high Da, although the LEM of Kerstein (1991) may be useful. [However, its successes are mixed.] The concept of LES that tracks the flame was suggested by analogy with the RVM and with adaptive grid methods. [Note: This has been suggested by others (random surface model) but still requires a model of the reaction zone and thus DNS coupled with flamelet or other models as appropriate.]
- All of the discussion centered on single-phase systems (conventional flames) since features of computational models in that area are amenable to testing by laboratory experiments and to some extent by DNS. A future challenge for DNS and

for theories with the same level of rigor as used in some of the models discussed here or studied in this workshop are flows with particulates (soot and ash formation, condensation reactions, spray combustion), radiation, wet combustion, and complex geometries with recirculation or backmixing.

4. Conclusions

In summary, F. Williams gave an overview of the regimes of applicability of the different types of combustion models, pointing out their shortcomings and the limitations of DNS for practical problems as well as the overriding importance of Da and Re in considering models for practical problems. S. B. Pope presented the case that one cannot do DNS for practical combustion systems but can learn something from simple canonical problems used for model building. T. Poinsot pointed out the difficulties with length and time scales in turbulent combustion but claims that DNS in premixed systems can be used for some practical combustion problems and has been used to validate the flamelet model.

Although the panel members were not in complete agreement, it is clear that there is a need for additional work on computational models and that DNS—even simplified canonical problems—can be useful for model development and validation and also for answering specific questions about the physics that are not accessible in the laboratory.

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