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A REVIEW OF MODERN DEVELOPMENTS IN LARGE EDDY SIMULATION OF TURBULENT REACTIVE FLOWS

PEYMAN GIVI

*Department of Mechanical and Aerospace Engineering
University at Buffalo, SUNY
Buffalo, NY 14260-4400*

Abstract. An overview is presented of recent developments and contributions in large eddy simulation (LES) of turbulent reactive flows. The foundation of some of the recently proposed subgrid scale (SGS) closures for such simulations is presented, along with a discussion of their capabilities and limitations. The scope of the review is limited to physical modeling. In doing so, only issues pertaining to additional complexities caused by chemical reactions are discussed. That is, the challenges associated with “general” LES of non-reactive flows are not considered, even though all of these challenges are indeed present (and in most cases are a lot more complex) in reactive flows. It is recognized that numerical algorithms and computational procedures play a significant role in (any) LES. However, this review does not deal with these issues except for cases wherein the actual numerical-computational methodology is directly coupled with the procedure by which LES is conducted. The SGS closure based on the recently developed “filtered density function” (FDF) method is described in a greater detail. This is due to more familiarity of this reviewer with this closure; it does not imply that other closures are less effective.

1. Introduction

In the late 1980's, I was preparing a review article on large scale numerical simulations of turbulent reactive flows. The intent was to provide a survey of the contributions made to both direct numerical simulation (DNS) and large eddy simulation (LES). However, when that article was finally published (Givi, 1989), its content was heavily biased towards DNS. This was not intentional, it just reflected the state of progress on LES of turbu-

lent combustion at that time. But with all of the enthusiasm for DNS in the combustion community, the limitations of such simulations were well recognized (even with the most optimistic predictions of growth in super-computer technology). It was also clear that the future of large scale simulations of practical turbulent reacting flows would heavily depend on the development of LES. Therefore, it was quite easy to predict that LES would receive significant attention in computational predictions of turbulent reacting flows in the 1990's and into the next (present) century.

Now, at the time of writing this article (Summer 2001), while struggling to meet the deadline for its submission(!) I am not surprised by the extent of the contributions in developing subgrid scale (SGS) models or by the magnificent work on LES of a variety of turbulent reacting flow systems. In fact, I admit that the rate of these developments has been a lot faster than my capability to absorb, or in some cases even follow, the details of the proposed methodologies. In addition, the page-limit restrictions under which this is being prepared, preclude describing the details of the wide variety of currently available closures; similarly, citation of the relevant references cannot even be done exhaustively. Fortunately, many aspects of SGS closures and LES of reacting turbulence have recently been discussed in several excellent tutorial and review articles (Cook and Riley, 1998a; Candel *et al.*, 1999; Bilger, 2000; Branley and Jones, 2000; Menon, 2000; Peters, 2000; Pope, 2000; Luo, 2001; Poinso and Veynante, 2001). Therefore, in the present review I concentrate on some of the major issues related to my area of research within this field.

2. Starting Equations

Large eddy simulation involves the use of the spatial filtering operation (Sagaut, 2001)

$$\langle Q(\mathbf{x}, t) \rangle_\ell = \int_{-\infty}^{+\infty} Q(\mathbf{x}', t) \mathcal{G}(\mathbf{x}', \mathbf{x}) d\mathbf{x}', \quad (1)$$

where \mathcal{G} denotes the filter function of width Δ_G , and $\langle Q(\mathbf{x}, t) \rangle_\ell$ represents the filtered value of the transport variable $Q(\mathbf{x}, t)$. In variable density flows it is convenient to consider the Favré filtered quantity,

$$\langle Q(\mathbf{x}, t) \rangle_L = \langle \rho Q \rangle_\ell / \langle \rho \rangle_\ell. \quad (2)$$

We consider spatially & temporally invariant and localized filter functions, $\mathcal{G}(\mathbf{x}', \mathbf{x}) \equiv G(\mathbf{x}' - \mathbf{x})$ with the properties $G(\mathbf{x}) = G(-\mathbf{x})$, and $\int_{-\infty}^{\infty} G(\mathbf{x}) d\mathbf{x} = 1$. Moreover, we only consider "positive" filter functions for which all the moments $\int_{-\infty}^{\infty} x^m G(x) dx$ exist for $m \geq 0$.

To set the framework, we consider the transport equations of chemically reacting flows. To isolate the effects of chemical reaction in the simplest way, we consider single-phase (gaseous) combustion in a low Mach number flow with negligible radiative heat transfer and viscous dissipation. We also assume that Newton's law of viscosity, Fourier's law of heat conduction and Fick's law of mass diffusion are applicable. Therefore, the primary transport variables are the density ρ , the velocity vector u_i , $i = 1, 2, 3$ along the x_i direction, the pressure p , the species' mass fractions Y_α , and the total specific enthalpy h . All of the mass fractions and the enthalpy are grouped into the scalar array $\phi(\mathbf{x}, t) \equiv [\phi_1, \phi_2, \dots, \phi_\sigma] \equiv [Y_1, Y_2, \dots, Y_{N_s}, h]$ of size $\sigma = N_s + 1$ where N_s denotes the total number of species. Application of the filtering operation to the equations of continuity, momentum, enthalpy (energy) and species mass fraction equations gives

$$\frac{\partial \langle \rho \rangle_\ell}{\partial t} + \frac{\partial \langle \rho \rangle_\ell \langle u_i \rangle_L}{\partial x_i} = 0, \quad (3)$$

$$\frac{\partial \langle \rho \rangle_\ell \langle u_j \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_\ell \langle u_i \rangle_L \langle u_j \rangle_L}{\partial x_i} = -\frac{\partial \langle p \rangle_\ell}{\partial x_j} + \frac{\partial \langle \tau_{ij} \rangle_\ell}{\partial x_i} - \frac{\partial T_{ij}}{\partial x_i}, \quad (4)$$

$$\frac{\partial \langle \rho \rangle_\ell \langle \phi_\alpha \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_\ell \langle u_i \rangle_L \langle \phi_\alpha \rangle_L}{\partial x_i} = -\frac{\partial \langle J_i^\alpha \rangle_\ell}{\partial x_i} - \frac{\partial M_i^\alpha}{\partial x_i} + \langle \rho S_\alpha \rangle_\ell, \quad (5)$$

where t represents time, and the filtered reaction source terms are denoted by $\langle \rho S_\alpha \rangle_\ell = \langle \rho \rangle_\ell \langle S_\alpha \rangle_L$. The viscous stress tensor and the mass/heat fluxes are denoted by τ_{ij} , and J_i^α , respectively. At low Mach numbers and heat release rates, by neglecting the viscous dissipation and thermal radiation the source terms in the enthalpy equation can be assumed to be negligible. Thus, $S_\alpha = S_\alpha(\phi)$. The terms $T_{ij} = \langle \rho \rangle_\ell (\langle u_i u_j \rangle_L - \langle u_i \rangle_L \langle u_j \rangle_L)$ and $M_i^\alpha = \langle \rho \rangle_\ell (\langle u_i \phi_\alpha \rangle_L - \langle u_i \rangle_L \langle \phi_\alpha \rangle_L)$ denote the SGS stress and the SGS mass flux, respectively. Equations (3)-(5) are coupled through the equation of state.

3. Closure Methodologies

For non-reacting flows the SGS closure is associated with T_{ij} and M_i^α (Canuto, 1994; Ciofalo, 1994; Lesieur and Metais, 1996). In reacting flows, an additional model is required for the filtered reaction rate $\langle S_\alpha \rangle_L$. This modeling is the subject of primary concern in this review.

One of the first contributions in LES of reactive flows, similar to that in LES of non-reacting flows, was made in atmospheric sciences (Schumann, 1989). In this work, the effects of SGS scalar fluctuations (as appear in the chemical source term) are assumed negligible, *i.e.* $\langle \hat{S}_\alpha(\phi) \rangle_L \approx \hat{S}_\alpha(\langle \phi \rangle_L)$. This assumption is compatible with that made in some of the more recent contributions (Boris *et al.*, 1992; Fureby and Grinstein, 1999), in which it

is argued that all of the essential SGS contributions are included in the numerical discretization procedure.

Modeling of the scalar fluctuations has been the subject of broad investigations in Reynolds averaged simulations (RAS) for over five decades, resulting in a variety of closure strategies (Libby and Williams, 1980; Libby and Williams, 1994). Within the past 10 years or so, almost all of these closures have been considered for LES. Examples: the eddy-break up models (Fureby and Lofstrom, 1994; Candel *et al.*, 1999), moment methods (Frankel *et al.*, 1993), the flamelet concept (Cook *et al.*, 1997; Cook and Riley, 1998b; De Bruyn Kops *et al.*, 1998; DesJardin and Frankel, 1998; DesJardin and Frankel, 1999; Pitsch and Steiner, 2000; Ladeinde *et al.*, 2001), the linear eddy model (LEM) (McMurtry *et al.*, 1992; Menon and Calhoon, 1996; Kim *et al.*, 1999; Menon, 2000), the conditional moment method (CMM) (Bushe and Steiner, 1999; Steiner and Bushe, 2001), and many others (Sykes *et al.*, 1992; Galperin and Orszag, 1993; Smith and Menon, 1996; Im *et al.*, 1997; McGrattan *et al.*, 1998; Thibaut and Candel, 1998; Battaglia *et al.*, 2000; Collin *et al.*, 2000). In addition, several of the closures previously developed for LES of non-reacting flows, have been extended for use in reacting flow simulations (DesJardin and Frankel, 1998; Jaber and James, 1998).

The probability density function (PDF) methods have proven particularly useful in RAS (O'Brien, 1980; Pope, 1985; Dopazo, 1994; Fox, 1996; Pope, 2000). The systematic approach for determining the PDF is by means of solving its transport equation. An alternative approach is based on *assumed* methods in which the shape of the PDF is specified *a priori*. This has been pursued in several studies in most of which it is assumed that the thermo-chemical variables depend only on the mixture fraction, *e.g.* infinitely fast reaction, equilibrium chemistry. Therefore, the PDF is univariate (Madnia and Givi, 1993; Cook and Riley, 1994; Réveillon and Vervisch, 1996; Branley and Jones, 1997; Jiménez *et al.*, 1997; Mathey and Chollet, 1997; DesJardin and Frankel, 1998; DesJardin and Frankel, 1999; Forkel and Janicka, 2000; Kempf *et al.*, 2000). For LES of non-equilibrium reactive flows, it is necessary to assume the joint PDF of multi-scalars (Frankel *et al.*, 1993). Consistent with popular methods of generating univariate (Leemis, 1986) and multivariate (Johnson and Kotz, 1972) distributions, all of the assumed SGS scalar PDFs in the contributions cited above are based on the first and the second order moments. The PDFs generated in this way offer sufficient flexibility and are affordable for large scale simulations. However, it is now well understood that the "true" PDF strongly depends on the actual physics of mixing in a given flow condition (Jaber *et al.*, 1996). Therefore, there is a need to determine such PDFs in a more systematic manner.

The “filtered density function” (FDF) methodology introduced by Pope (1990) provides the framework for fundamental developments of the PDF based SGS closures. This method provides a means of determining the PDF from its own transport equation. For the scalars’ array $\phi(\mathbf{x}, t)$ the FDF, denoted by P_L , is defined as (Pope, 1990)

$$P_L(\psi; \mathbf{x}, t) = \int_{-\infty}^{+\infty} \zeta[\psi, \phi(\mathbf{x}', t)] G(\mathbf{x}' - \mathbf{x}) d\mathbf{x}', \quad (6)$$

$$\zeta[\psi, \phi(\mathbf{x}, t)] = \prod_{\alpha=1}^{\sigma} \delta[\psi_{\alpha} - \phi_{\alpha}(\mathbf{x}, t)], \quad (7)$$

where δ denotes the delta function and ψ denotes the composition domain of the scalar array. The term $\zeta[\phi - \psi(\mathbf{x}, t)]$ is the “fine-grained” density (Lundgren, 1967; O’Brien, 1980; Pope, 1985; Dopazo, 1994). In variable density flows, it is convenient to consider the “filtered mass density function” (FMDF), denoted by F_L , as

$$F_L(\psi; \mathbf{x}, t) \equiv \int_{-\infty}^{+\infty} \rho(\mathbf{x}', t) \zeta[\psi, \phi(\mathbf{x}', t)] G(\mathbf{x}' - \mathbf{x}) d\mathbf{x}'. \quad (8)$$

The integral property of the FDF and FMDF is such that

$$\int_{-\infty}^{+\infty} P_L(\psi; \mathbf{x}, t) d\psi = 1, \quad \int_{-\infty}^{+\infty} F_L(\psi; \mathbf{x}, t) d\psi = \langle \rho(\mathbf{x}, t) \rangle_{\ell}. \quad (9)$$

For further discussions, it is useful to define the mass weighted conditional filtered mean of the variable $Q(\mathbf{x}, t)$,

$$\langle Q(\mathbf{x}, t) | \psi \rangle_{\ell} \equiv \frac{\int_{-\infty}^{+\infty} \rho(\mathbf{x}', t) Q(\mathbf{x}', t) \zeta[\psi, \phi(\mathbf{x}', t)] G(\mathbf{x}' - \mathbf{x}) d\mathbf{x}'}{F_L(\psi; \mathbf{x}, t)}. \quad (10)$$

Therefore, when Q can be completely described by the compositional variable, *i.e.* $Q(\mathbf{x}, t) \equiv \hat{Q}(\phi(\mathbf{x}, t))$, we have $\langle Q(\mathbf{x}, t) | \psi \rangle_{\ell} = \hat{Q}(\psi)$. Also,

$$\int_{-\infty}^{+\infty} \langle Q(\mathbf{x}, t) | \psi \rangle_{\ell} F_L(\psi; \mathbf{x}, t) d\psi = \langle \rho(\mathbf{x}, t) \rangle_{\ell} \langle Q(\mathbf{x}, t) \rangle_L. \quad (11)$$

The transport equation for $F_L(\psi; \mathbf{x}, t)$ is obtained by multiplying the transport equation for the fine grained density by the filter function $G(\mathbf{x}' - \mathbf{x})$ and integrating over \mathbf{x}' space (Gao and O’Brien, 1993; Colucci *et al.*, 1998; Réveillon and Vervisch, 1998; Jaber *et al.*, 1999; Jaber, 1999; Zhou and Pereira, 2000; Tong, 2001),

$$\frac{\partial F_L(\boldsymbol{\psi}; \mathbf{x}, t)}{\partial t} + \frac{\partial[\langle u_i(\mathbf{x}, t) | \boldsymbol{\psi} \rangle_\ell F_L(\boldsymbol{\psi}; \mathbf{x}, t)]}{\partial x_i} = - \frac{\partial[\hat{S}_\alpha(\boldsymbol{\psi}) F_L(\boldsymbol{\psi}; \mathbf{x}, t)]}{\partial \psi_\alpha} + \frac{\partial}{\partial \psi_\alpha} \left[\left\langle \frac{1}{\hat{\rho}(\phi)} \frac{\partial J_i^\alpha}{\partial x_i} | \boldsymbol{\psi} \right\rangle_\ell F_L(\boldsymbol{\psi}; \mathbf{x}, t) \right]. \quad (12)$$

The first term on the RHS is due to chemical reaction and is in a closed form. This demonstrates the primary advantage of the FDF methodology. However, the SGS convection (the second term on the LHS) and SGS mixing (the second term on the RHS) must be modeled. One of the most challenging issues in FDF is associated with closure of the mixing term. This has been the subject of broad investigations in PDF modeling (Pope, 1985; Pope, 2000). In Eq. (12) the effects of mixing are displayed through the “conditional expected diffusion” of the scalars, but can also be represented in the form of the “conditional expected dissipation” (O’Brien, 1980; Pope, 1985). The closure for this can be via any of the ones currently in use in PDF methods (Pope, 2000). In the absence of a clearly superior model, the linear mean square estimation (LMSE) model (O’Brien, 1980) has been used in almost all of previous LES based on FDF (Colucci *et al.*, 1998; Jaber *et al.*, 1999; Garrick *et al.*, 1999; James and Jaber, 2000; Zhou and Pereira, 2000). With $J_i^\alpha = -\gamma \frac{\partial \phi_\alpha}{\partial x_i}$, this model is

$$\frac{\partial}{\partial \psi_\alpha} \left[\left\langle -\frac{1}{\hat{\rho}} \frac{\partial}{\partial x_i} \left(\gamma \frac{\partial \phi_\alpha}{\partial x_i} \right) | \boldsymbol{\psi} \right\rangle_\ell F_L \right] = \frac{\partial}{\partial x_i} \left[\gamma \frac{\partial (F_L / \langle \rho \rangle_\ell)}{\partial x_i} \right] + \frac{\partial}{\partial \psi_\alpha} [\Omega_m(\psi_\alpha - \langle \phi_\alpha \rangle_L) F_L], \quad (13)$$

where $\Omega_m(\mathbf{x}, t)$ is the “frequency” of mixing within the subgrid and must be modeled. The convective term can be modeled as

$$\langle u_i | \boldsymbol{\psi} \rangle_\ell F_L = \langle u_i \rangle_L F_L - \gamma_t \frac{\partial (F_L / \langle \rho \rangle_\ell)}{\partial x_i}, \quad (14)$$

where γ_t is the SGS diffusion coefficient and must be specified. Equation (14) is in accord with that often used in conventional LES (Moin *et al.*, 1991; Canuto, 1994; Ciofalo, 1994; Lesieur and Metais, 1996). With this formulation, obviously the resolved hydrodynamic field must be determined by other means. This problem can be circumvented by considering the joint velocity-scalar FMDF,

$$\mathcal{F}_L(\mathbf{v}, \boldsymbol{\psi}, \mathbf{x}; t) \equiv \int_{-\infty}^{+\infty} \rho(\mathbf{x}', t) \xi[\mathbf{v}, \mathbf{u}(\mathbf{x}', t), \boldsymbol{\psi}, \phi(\mathbf{x}', t)] G(\mathbf{x}' - \mathbf{x}) d\mathbf{x}', \quad (15)$$

$$\xi[\mathbf{v}, \mathbf{u}(\mathbf{x}, t), \boldsymbol{\psi}, \boldsymbol{\phi}(\mathbf{x}, t)] = \prod_{k=1}^3 \delta[v_k - u_k(\mathbf{x}, t)] \prod_{\alpha=1}^{\sigma} \delta[\psi_{\alpha} - \phi_{\alpha}(\mathbf{x}, t)], \quad (16)$$

where \mathbf{v} denotes the composition domain of the random velocity vector, and $\xi[\mathbf{v}, \mathbf{u}(\mathbf{x}, t), \boldsymbol{\psi}, \boldsymbol{\phi}(\mathbf{x}, t)]$ is the fine-grained velocity-scalar density. Most recent work in this regard consider the transport of the velocity FDF (VFDF) (Gicquel, 2001) and the joint velocity-scalar FDF (VSFDF) (Drozda, 2001). The operational procedure is similar to that developed previously for PDF methods (Pope, 1985; Pope, 1994; Pope, 2000).

The closure problems as noted above are not particular to the FDF; all of the other schemes require similar modelings. For example, in the limit of equilibrium chemistry all of the statistics of the reacting fields are related to those of the mixture fraction. The FMDF of the mixture fraction can be obtained from the solution of Eq. (12) with $S = 0$. So, there is still a need for modeling of the mixing term. Even in cases where the FMDF is assumed, its distribution is parameterized with the low order moments of the mixture fraction. As indicated above, the first two moments are typically used for this parameterization. Therefore, there is a need for closure of the “total SGS dissipation” as appears in the second moment (SGS variance) equation. Several means of dealing with this closure problem are available (Girimaji and Zhou, 1996; Pierce and Moin, 1998; Cook and Bushe, 1999; Jiménez *et al.*, 2001; De Bruyn Kops and Riley, 2001).

The above problem is a bit more complex when the SGS chemical reaction is assumed to be in the “flamelet” regime (Peters, 2000). In this case, even with the one-dimensional flamelet model, the thermo-chemical variables are parameterized by the mixture fraction and its rate of dissipation (Cook *et al.*, 1997; Cook and Riley, 1998b; De Bruyn Kops *et al.*, 1998; DesJardin and Frankel, 1998; Cook and Riley, 1998b). Therefore, there is a need for *a priori* specification of the joint FDF of the mixture fraction and its dissipation. A review of different methods of dealing with this issue is available (Cook and Riley, 1998a). Equation (12) with $S = 0$ indicates that there is a dependence between the FDF of the mixture fractions and the conditional expected diffusion (and the conditional expected dissipation). This dependency is not considered in most previous contributions, but is the subject of current investigations (DesJardin *et al.*, 2001).

Modeling of the conditional expected dissipation is also required in the conditional moment method (Bushe and Steiner, 1999; Steiner and Bushe, 2001). This issue has been recognized at the early stages of developments of CMM in RAS (Bilger, 2000). With this model, the conditional filtered mean values of the thermo-chemical variables (LHS of Eq. (10)) are obtained by their modeled transport equation. This is obviously computationally less demanding than solving the FDF transport equation. But in order to

determine the actual filtered quantities, the distribution of the mixture fraction FDF must be specified.

An important issue in regard to FDF is associated with the numerical solution of its transport equation. The Lagrangian Monte Carlo scheme (Pope, 1985) has proven particularly useful for this purpose. In this scheme, the FDF is represented via an ensemble of computational elements or particles. Transport of these particles and the change in their properties are modeled by a set of stochastic differential equations (SDEs) (Soong, 1973). The diffusion process (Gardiner, 1990) has proven effective for this purpose. The coefficients in the Langevin equation governing this process are set in such a way that the resulting Fokker-Planck equation (Risken, 1989) is equivalent to the FDF transport equation. Therefore, the Monte Carlo solution of the SDEs represent the solution of the FDF in the probabilistic sense. This procedure has proven successful for simulating PDF in a variety of systems (Grigoriu, 1995). However, one must be careful in performing stochastic simulations in conjunction with modern CFD solvers. Many of the advanced discretization routines developed for solving deterministic differential equations may not be applicable, or may have to be significantly modified to be suitable for solving SDEs (Kloeden and Platen, 1995).

Implementation of LEM is also based on stochastic representation of the flow. In its original development in RAS (Kerstein, 1988), the processes of molecular diffusion, chemical reaction and turbulent convection are considered separately. This is achieved by a reduced one-dimensional (linear) description of the scalar field, which makes it possible to resolve the flow scales even for flows with relatively high Reynolds, Schmidt and Damköhler numbers. The interpretation of the one-dimensional domain is dependent on the particular flow under consideration. In this way, the processes of molecular diffusion and chemical reaction are taken into account exactly, but the effects of convection are modeled. This is achieved by "random rearrangement" (or stirring) events in such a way that the displacements of fluid elements result in a diffusivity equal to the "turbulent diffusivity." For LES, this procedure is followed within each of the computational cells, and stirring is performed to yield the desired SGS diffusivity. Menon and colleagues have made extensive use of LEM for LES of a wide variety of reacting flows. A recent review is available (Menon, 2000).

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