LES of non-premixed turbulent reacting flows with Conditional Source term Estimation

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1. Motivation and objectives

In the foreseeable future, Direct Numerical Simulation (DNS), a technique in which all flow scales are resolved, will remain computationally unaffordable for turbulent reacting flows at technically relevant high Reynolds numbers Thus, Large Eddy Simulation (LES), which resolves only the large scale motion of the flow while modeling the contribution of the small (subgrid) scales, has been recognized as a powerful alternative approach. The LES set of equations is obtained by applying a spatial filter to the governing transport equations of mass, momentum, and energy. Several subgrid-scale models for the filtered means of the unresolved turbulent transport of momentum and species have been developed. They range from the widely used constant-coefficient model of Smagorinsky (1963) to dynamic models where the model coefficients are computed as functions of the instantaneous flow field (Moin *et al.*, 1991; Germano *et al.*, 1991). These dynamic models, which have proven to be successful in many types of non-reacting flows, are well established tools in LES. In combusting flows, however, the subgrid-scale modeling of the chemistry is still a major challenge; our present study is focused on this issue.

In an LES of turbulent reactive flows, a spatial filter is applied to the governing set of differential conservation equations. Let

$$\widetilde{f} = \frac{\overline{\rho f}}{\overline{\rho}}$$

be the density weighted (or Favre) filtered representation of some quantity f. Then, the filtered transport equations for the mass fraction Y_I of some species I and enthalpy $\widetilde{h} = \overline{c}_p \widetilde{T}$ read

$$\frac{\partial \overline{\rho} \widetilde{Y}_I}{\partial t} + \frac{\partial \overline{\rho} \widetilde{u}_i \widetilde{Y}_I}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\overline{\rho} \left(\widetilde{\mathcal{D}}_l + \widetilde{\mathcal{D}}_t \right)_I \frac{\partial \widetilde{Y}_I}{\partial x_i} \right] + \overline{\dot{\omega}}_I, \tag{1}$$

$$\frac{\partial \overline{\rho} \widetilde{h}}{\partial t} + \frac{\partial \overline{\rho} \widetilde{u}_i \widetilde{h}}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\overline{\rho} \left(\widetilde{\kappa}_l + \widetilde{\kappa}_t \right) \frac{\partial \widetilde{T}}{\partial x_i} \right] + \sum_I (\overline{\dot{\omega}}_I h_{0_I}), \tag{2}$$

where $\overline{\rho}$ is the spatially filtered density and $\overline{\dot{\omega}}_I$ and h_{0_I} are the reactive source term and the enthalpy of formation of species I, respectively. The turbulent subgrid-scale fluxes

$$\overline{\rho} \left(\widetilde{u}_i \widetilde{Y}_I - \widetilde{u_i Y_I} \right) = \overline{\rho} \widetilde{\mathcal{D}}_{t_I} \frac{\partial \widetilde{Y}_I}{\partial x_i}$$

$$\overline{\rho}\left(\widetilde{u_i}\widetilde{h} - \widetilde{u_i h}\right) = \overline{\rho}\widetilde{\kappa}_t \frac{\partial \widetilde{T}}{\partial x_i}$$

have been modeled in terms of diffusive fluxes involving the corresponding eddy diffusivities $\widetilde{\mathcal{D}}_{tI}$ and $\widetilde{\kappa}_t$. Subgrid-scale models providing these quantities have already been mentioned above.

The main challenge faced in modeling combustion is that chemical reaction rates are usually highly non-linear functions of temperature, density, and species mass fractions. For a system with N possible species, the K-th chemical reaction can be written as

$$\sum_{J=1}^{N} \eta'_{JK} A_J \rightleftharpoons \sum_{J=1}^{N} \eta''_{JK} A_J,$$

where A_J is the chemical symbol for species J and η'_{JK} and η''_{JK} are the stoichiometric coefficients for species J in reaction K. If M chemical reactions are to be considered, then the chemical source term for species I becomes (Williams, 1985)

$$\dot{\omega}_I = W_I \sum_{K=1}^{M} (\eta''_{IK} - \eta'_{IK}) B_K T^{\gamma_K} e^{-\frac{E_K}{RT}} \prod_{J=1}^{N} \left(\frac{\rho Y_J}{W_J}\right)^{\eta'_{JK}}, \tag{3}$$

where W_I is the molecular mass of species I, T is the temperature, R is the universal ideal gas constant, E_K is the activation energy, and B_K is the frequency factor. The power of the pre-exponential term γ_K for reaction K accounts for non-exponential temperature dependence of the reaction rate. Due to the strong non-linearity of (3), substituting the filtered temperature, density, and mass fractions into (3), yielding

$$\overline{\dot{\omega}_I} \approx \dot{\omega}_I(\overline{\rho}, \widetilde{T}, \widetilde{Y_J}),$$

will generally provide a very poor estimate for the filtered reaction rates. It is evident that closure for the filtered chemical reaction rates has to be provided. In non-premixed combustion, where fuel and oxidizer are initially separated and must mix together before they react, several different approaches have been suggested:

Assuming Fast Chemistry circumvents the estimation of the chemical source terms. Under this assumption the thermodynamical state is completely determined as a function of the mixture fraction (Cook & Riley, 1994). However, effects like ignition and extinction, which may crucially affect many real flames, cannot be accounted for. Fast Chemistry also poorly predicts pollutants whose rates of formation are kinetically limited.

The Laminar Flamelet model (Peters, 1984; Cook *et al.*, 1997) assumes the flame structures to be thin in comparison to the turbulent eddies. Within the "laminar flamelet regime" the flame is considered to be comprised of an ensemble of strained laminar flames, which themselves merely depend on mixture fraction and scalar dissipation. Given the filtered means of these two quantities and assuming the shape of their joint probability density function, the filtered means of the mass fractions and temperature can be computed. There is still considerable argument on the

applicability of this method to flames outside the "flamelet regime". Furthermore, the chemistry is assumed to be in steady-state; for LES, this implies a quasi-steady-state assumption neglecting important transient effects on phenomena like ignition and extinction. In order to overcome this drawback, an unsteady Laminar Flamelet model has been devised for RANS of combusting flows (Peters, 1997). Thereby, an unsteady flamelet code is running simultaneously with the CFD code. Receiving the time dependent thermodynamic state and the scalar dissipation from the CFD code as inputs, the unsteady flamelet solution yields the actual chemical composition as a function of mixture fraction. Assuming the shape of the probability density function for the mixture fraction, the updated chemical composition vector in physical space can be computed and fed into the CFD code. Whether or not the unsteady Laminar Flamelet model can also be employed in LES has yet to be investigated. Unlike unsteady RANS, LES provides a time-accurate solution without periodicity in time. Thus, the number of unsteady flamelets to be tracked might increase continuously; in the long run, this could make the LES prohibitively expensive.

The PDF-Transport methods solve a transport equation for the Filtered Joint Probability Density Function of mass fractions, energy, etc. (Pope 1985; Givi, 1989; Colucci *et al.*, 1998). In the transport equation of the PDF, the chemical source terms occur in closed form; however, the dimensionality increases with the number of species, and the unclosed molecular mixing term has to be modeled. The closure problem for the chemical reaction term has apparently been commuted to the closure for the molecular mixing.

Recently, Bilger (1993a,1993b) and Klimenko (1990) independently proposed a new approach for modeling turbulent reacting flows, called Conditional Moment Closure (CMC). The CMC method solves for the transport equations of conditionally averaged quantities instead of their spatially filtered counterparts. Variables on which the chemical reactions are known to depend on are chosen to be the conditioning variables. Solving the transport equations also in conditioning space adds a further dimension to the problem which inhibits the application of CMC to three-dimensional flow simulations due to its high computational cost.

In the present study the Conditional Source term Estimation (CSE) method (Bushe & Steiner, 1998) has been proposed as an alternative to the aforementioned methods for closing the chemical source terms. CSE is based on the CMC hypothesis. However, unlike in traditional CMC methods, it is not necessary to solve the transport equations in the conditioning space; this makes the method computationally affordable. In its present form the proposed model is devised to provide the filtered means of the chemical source terms needed to close the LES set of equations in reacting flows. CSE has proven its predictive capability in an *a priori* test using DNS data of turbulent reacting mixing layer, and it is currently being tested in an LES of a turbulent jet diffusion flame.

2. Accomplishments

2.1 Conditional Source term Estimation (CSE)

CSE is based on the CMC closure hypothesis. In the CMC method proposed

by Klimenko (1990) and Bilger (1993a, 1993b), the transport equations are conditionally averaged, with the condition being some variable on which the chemical reaction rates are known to depend.

2.2.1 One condition

In non-premixed combustion far from extinction, the reaction rates mainly depend on mixture fraction. Thus, the mixture fraction is clearly an appropriate conditioning variable. In the context of non-premixed combustion, the mixture fraction represents the local fraction of mass originating from the feeding fuel stream. Thus, it is zero in pure oxidizer and one in pure fuel. In the following the conditional average of some quantity f, conditional on the mixture fraction Z having some value ζ, will be denoted by an overline:

$$\overline{f \mid Z} = \langle f \mid Z = \zeta \rangle.$$

The conditionally averaged reaction term occurring in the conditionally averaged transport equation for the mass fraction Y_I is closed with the first order CMC hypothesis: the conditional average of the chemical source term of some species I can be modeled by evaluating the chemical reaction rates using the conditional averages of the composition vector $\overline{Y_K \mid Z}$, temperature $\overline{T \mid Z}$, and density $\overline{\rho \mid Z}$. Thus,

$$\overline{\dot{\omega}_I(Y_K, T, \rho) \mid Z} \approx \dot{\omega}_I \left(\overline{Y_K \mid Z}, \overline{T \mid Z}, \overline{\rho \mid Z} \right). \qquad (4)$$

It has been established that the CMC hypothesis, based on a single conditioning variable, provides adequate predictions of reaction rates for flames far from extinction (Bilger, 1993a; Smith 1994). The CSE method makes use of the CMC hypothesis (4); however, it suggests an alternative way to obtain the conditional averages. Rather than solving the conditionally averaged transport equations, which would be computationally expensive having the mixture fraction Z as additional dimension, it takes advantage of the spatial homogeneity of the conditional averages on particular surfaces in the reacting flow field. For example, in case of a reacting mixing layer, the conditionally averaged quantities show only small variation on planes normal to the reacting interface. Based on this spatial homogeneity the "extraction" process of the conditional averages might work as follows: For some set of $m = 1, ..., M$ cells in an LES domain which lie on the surface of homogeneity, the conditional average of the temperature is invariant in all m cells:

$$\left(\overline{T \mid Z} \right)_m = \overline{T \mid Z}. \qquad (5)$$

The density weighted, filtered temperature in each cell m can be expressed as

$$\overline{T}_m = \int_0^1 P_m(Z) \, \overline{T \mid Z} \, dZ, \qquad (6)$$

where $P_m(Z)$ is the probability density function of the mixture fraction within the filtered cell m. Eq. (6) is an integral equation—a Fredholm equation of the first

kind—which, for discrete intervals in Z, can be inverted to yield $\overline{T\,|\,Z}$. Similar equations can be written for the density and the mass fractions to obtain $\overline{\rho\,|\,Z}$ and $\overline{Y_K\,|\,Z}$, respectively . Even in the case of non-homogeneity, where (5) does not hold, the inversion of (6) would still yield an approximation for the conditional average of the temperature on the surface constituted by the ensemble of $m = 1, ..., M$ LES cells. The conditional average of the chemical source terms $\overline{\dot{\omega}_I\,|\,Z}$ can now be obtained using the CMC hypothesis (4), and the unconditional mean chemical source term is then

$$\overline{\dot{\omega}}_{I,m} = \int_0^1 P_m(Z)\ \overline{\dot{\omega}_I\,|\,Z}\ dZ. \tag{7}$$

In this manner, it should be possible to obtain closure for the sub-grid scale mean reaction rate for any chemical kinetic mechanism. No assumptions have been made regarding the thickness of the regions in which chemical reactions are significant relative to the turbulent length scales. Only the assumption of statistical homogeneity of the conditional averages of temperature, density, and pressure on some surface must be made. As for the probability density function $P_m(Z)$, a $\beta-PDF$ with the same mean $\overline{Z}_m$ and variance $\overline{Z'^2_m}$ of the mixture fraction has proven to approximate the real PDF appropriately (Bushe & Steiner, 1998). The mean of the mixture fraction $\overline{Z}_m$ is obtained as a resolved quantity of the LES. The filtered variance $\overline{Z'^2_m}$ can be estimated either through a subgrid-scale model, e.g., a Dynamic Model or using a similarity approach (Jiménez *et al.*, 1996), or by solving a transport equation for $\overline{Z'^2_m}$. The latter, however, requires modeling of the filtered scalar dissipation

$$\overline{\chi} = \overline{2\rho\nabla Z\nabla Z}. \tag{8}$$

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2.2.1 Two conditions

It is known that conditioning only on mixture fraction is insufficient to account for phenomena such as extinction or ignition. Since the occurrence of these phenomena depends strongly on the scalar dissipation χ, defined in (8), it seems sensible to introduce scalar dissipation—or some closely related quantity—as the additional conditioning variable (Bushe, 1995). Assuming for the functional dependence of scalar dissipation on mixture fraction the shape of the laminar counter-flow solution (Peters, 1984), the scalar dissipation can be written as

$$\chi = \chi^* \cdot \exp\left(-2\left[\mathrm{erf}^{-1}(Z)\right]^2\right). \tag{9}$$

The sufficiently weak dependence of the new random variable χ^* on the mixture fraction Z allows expression of the joint probability density function $P(Z, \chi^*)$ as

$$P(Z, \chi^*) = P(Z)\, P(\chi^*),$$

where $P(Z)$ again can be approximated as a $\beta-PDF$. Analogously to the assumptions made for PDF of the scalar dissipation χ (Monin & Yaglom, 1975; Eswaran

& Pope, 1988; Yeung & Pope 1989), the probability density function of χ^* is taken to be approximately log-normal as well. In every LES cell m, $P_m(\chi^*)$ is determined in terms of the filtered mean $\overline{\chi^*}_m$ and the standard deviation. The first is provided by the relation

$$\overline{\chi}_m = \int_0^1 P_m(Z) \, \overline{\chi \,|\, Z} dZ = \overline{\chi^*}_m \int_0^1 P_m(Z) \cdot \exp\left(-2\left[\mathrm{erf}^{-1}(Z)\right]^2\right) dZ, \qquad (10)$$

and the latter is taken to be unity. The rhs of (10) involves again a $\beta - PDF$ for $P_m(Z)$ and the laminar counter-flow solution. The filtered mean of the scalar dissipation $\overline{\chi}_m$ has to be modeled.

The "extraction" process of the conditional averages is then straightforward. It is virtually the same as already described for one condition in the previous section. Inverting the expression

$$\overline{T}_m = \int_0^\infty \int_0^1 P_m(Z, \chi^*) \, \overline{T \,|\, Z, \chi^*} \, dZ \, d\chi^*, \qquad (11)$$

which is equivalent to (6) in the one-condition case, yields the conditionally averaged quantities needed for the CMC hypothesis now with two conditions:

$$\overline{\dot{\omega}_I \,|\, Z, \chi^*} \approx \dot{\omega}\left(\overline{Y_K \,|\, Z, \chi^*}, \overline{T \,|\, Z, \chi^*}, \overline{\rho \,|\, Z, \chi^*}\right). \qquad (12)$$

The mean chemical source term becomes

$$\overline{\dot{\omega}}_{I,m} = \int_0^\infty \int_0^1 P_m(Z, \chi^*) \, \overline{\dot{\omega}_I \,|\, Z, \chi^*} \, dZ \, d\chi^*. \qquad (13)$$

2.2.3 Effects of density weighted filtering

Dealing with non-constant density flows the LES set of transport equations (1)-(2) are solved for the Favre filtered averages of mass fractions and temperature. In this case the CSE equations have only to be adjusted to the density weighted LES inputs into the model, the closure hypothesis and the extraction process remain the same. In terms of density weighted averages (6) and (7) read

$$\widetilde{T}_m = \int_0^1 \widetilde{P}_m(Z) \, \overline{T \,|\, Z} \, dZ,$$

$$\overline{\dot{\omega}}_m = \overline{\rho}_m \int_0^1 \widetilde{P}_m(Z) \, \overline{\dot{\omega} \,|\, Z} \left(\overline{\rho \,|\, Z}\right)^{-1} \, dZ,$$

respectively, where $\widetilde{P}_m(Z) = P(Z; \widetilde{Z}_m, \widetilde{Z''^2_m})$ is the Favre PDF of the mixture fraction, which will again be approximated using the β-PDF. Its shape is now determined by the Favre filtered mean and variance of the mixture fraction $\widetilde{Z}_m$ and $\widetilde{Z''^2_m}$, respectively.
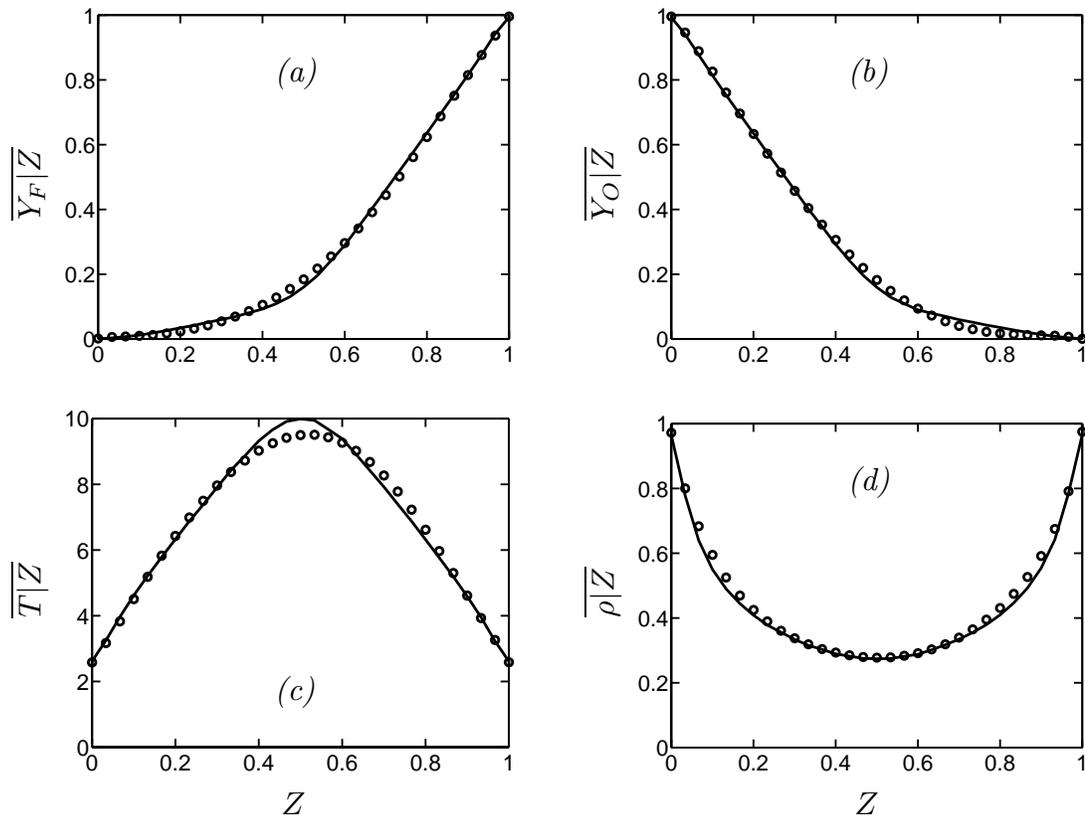
FIGURE 1.   Result of *a priori* test of integral inversion process to obtain the conditional averages of: *(a)* mass fraction of fuel, *(b)* mass fraction of oxidizer, *(c)* non-dimensional temperature, *(d)* non-dimensional density; ——— : result of inversion process, ∘ : DNS value.

2.3 A priori test of the model

In order to test the method described above, the output from several different time steps in the DNS database of Vervisch (1992) was filtered. The simulation is of a shear-free, temporal mixing layer with fuel and oxidizer mixing in the presence of turbulence. The domain was rectangular with 128 points across the layer and 64 points in each direction tangential to the layer. A $(16 \times 8 \times 8)$−top-hat filter was used to compute the spatially filtered means on the LES grid.

The chemical kinetic mechanism used in creating the DNS database was a single step,

$$F + O \rightarrow P,$$

with F, O, and P being Fuel, Oxidizer, and Product, respectively. The reaction rate was

$$\dot{\omega} = Da \, \rho^2 \, Y_F \, Y_O \, \exp\left(\frac{-\beta(1-\theta)}{1-\alpha(1-\theta)}\right),$$

with

$$\alpha = \frac{T_{\mathrm{ad}} - T_0}{T_{\mathrm{ad}}} = 0.8\,, \quad \beta = 8 \quad \text{and} \quad \theta = \frac{T - T_0}{T_0 - T_{\mathrm{ad}}}\,.$$
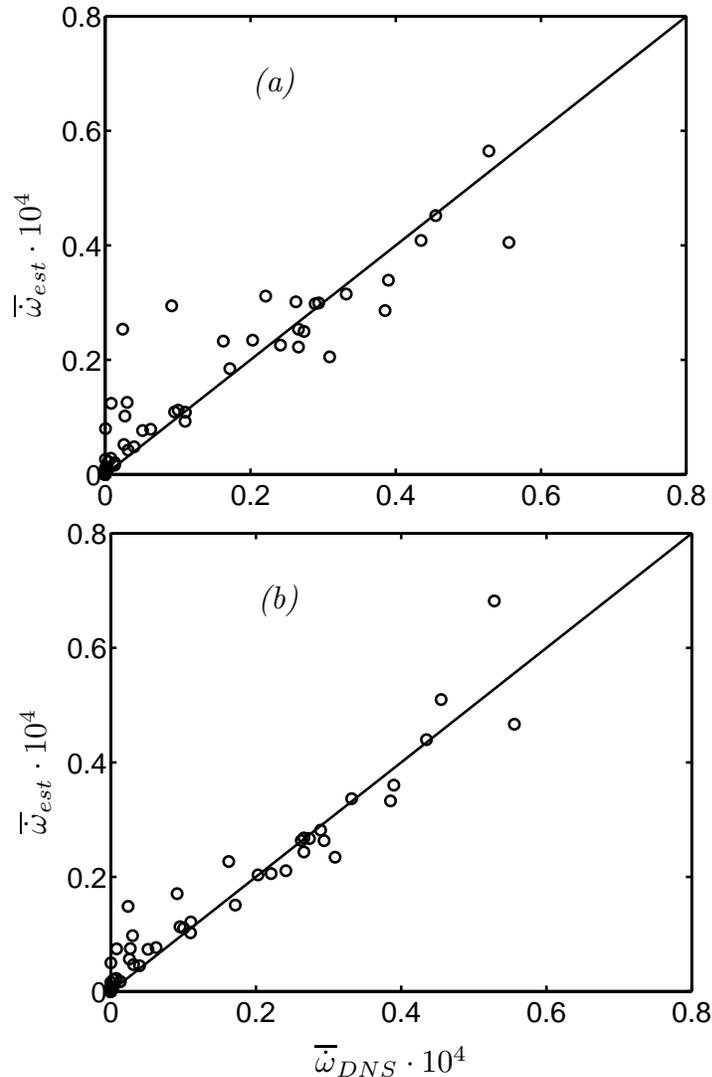
FIGURE 2. Comparison of reaction rate $\overline{\dot{\omega}}_{est}$ estimated using CSE closure to filtered reaction rate from DNS data $\overline{\dot{\omega}}_{DNS}$: *(a)* CSE with one conditioning variable Z, *(b)* CSE with two conditioning variables Z and χ^*.

All temperatures—including T_0 (the initial temperature) and T_{ad} (the adiabatic flame temperature at stoichiometric conditions)—were non-dimensionalized with the reference temperature $T_{ref} = (\gamma - 1) T_0$, and γ, the ratio of specific heats, was taken to be 1.4. The Damköhler number Da was unity.

The first test was to try to use the quantities $\overline{Z}_m$ and $\overline{Z'^2_m}$ at each point to predict $P_m(Z)$ using the β−PDF as described above and then to substitute $\overline{\rho}_m$, $\overline{Y_{Fm}}$, $\overline{Y_{Om}}$, and $\overline{T}_m$ and $P_m(Z)$ into (6) to predict the conditional averages. The results of this *a priori* test for one time in the simulation (a fairly late time, approximately 1.6 eddy turnover times in the simulation) are shown in Fig. 1, where the results of the inversion of the integral equation using a simple linear regularization method is compared to the actual conditional average from the entire flow field. With the

exception of a slight over-prediction of the maximum temperature, the prediction of the conditional averages appears to be very good. Similar results have been found for all other times at which data is available.

The next test is to invoke the CMC hypothesis (4) and use these conditional averages to predict the conditional mean reaction rate $\overline{\dot{\omega} \,|\, Z}$. Then, the unconditional mean reaction rate is predicted from the prediction of the conditional mean reaction rate using (7). The estimate $\overline{\dot{\omega}}_{est}$ obtained by this process is compared to the actual average of the reaction rate $\overline{\dot{\omega}}_{DNS}$ in every cell in Fig. 2a. The standard error in the prediction of the cells where $\overline{\dot{\omega}}_{DNS}$ is significant (greater than 1×10^{-5}) is about 15%. It should be noted that there is some extinction in the DNS database which cannot be predicted by the single condition version of this method. This is made evident by the presence of several points where $\overline{\dot{\omega}}_{DNS}$ is very small but $\overline{\dot{\omega}}_{est}$ is still significant. These are cells which contain local extinction events. Nevertheless, that the method is capable of predicting the reaction rates with such accuracy even in the presence of heat release and extinction seems to be very encouraging.

As was discussed above, adding a second condition to the inversion process is expected to make the method capable of modeling extinction and ignition phenomena. This was tested by simply adding the second condition and inverting the two-dimensional problem described by (11), using the conditional averages to estimate the conditional average of the reaction rate (12) and integrating (13). The result of this process is shown in Fig. 2b. The standard error in the prediction of the cells where $\overline{\dot{\omega}}_{DNS}$ is significant (again, greater than 1×10^{-5}) is about 10%. Not only is the error in the prediction somewhat smaller than was found with only one condition, the evidence of over-prediction of the reaction rate in cells containing extinction events is no longer apparent. It seems that the extinction phenomenon is captured at least to some extent by the inclusion of the second conditioning variable. Thus, even though the overall improvement of the prediction for the reaction rate at first sight seems to be rather small, the additional effort of carrying a second condition variable is still justified: it makes it possible to account for extinction and ignition phenomena.

Future plans

The CSE model is at present being tested in an LES of turbulent reacting jets. The code into which the subgrid-scale models have been introduced originally was written for DNS of non-reacting jets by Boersma (1998a). The first test considers a piloted jet diffusion flame at $Re = 4000$; for this basic test case one-step chemistry is assumed. Preliminary results of this LES showing temperature and fuel mass fraction contours when looking at the vertical jet from the side are presented in Fig. 3. Planes of equal distance downstream from the nozzle exit have been assumed as statistically homogeneous surfaces. The conditional averages have been computed using the LES filtered means gathered on these planes. The LES results obtained so far are going to be compared with the corresponding DNS data. These DNS data will be provided by a DNS performed by Boersma (1998b) for exactly the same test case. Further test cases will then consider experimentally investigated methane-air flames with high Reynolds numbers. The first case will deal with a piloted

<center>(a) (b)</center>

FIGURE 3. Results of LES of piloted jet flame: *(a)* non-dimensional temperature: white-black, $T/T_0 = 1$ to 5; *(b)* mass fraction of fuel: white-black, $Y_F = 0$ to 1.

jet flame experiment performed in the Sandia Turbulent Diffusion Flame Facility (Masri *et al.*, 1988a,1988b). From these measurements extensive data on chemical composition and temperature fields are available. Then LES of a lifted methane-air jet (Muñiz & Mungal, 1997) will be attempted. There, the main challenge will be to capture ignition effects. Using a second conditioning variable, it is hoped that it will be possible to obtain a realistic prediction for the flame liftoff heights.

Acknowledgments

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