

# Direct numerical simulation of turbulent premixed flames with a marker field and application to RANS and LES

By R. W. Bilger †, S. H. Kim AND S.M. Martin

Direct numerical simulations of turbulent premixed combustion in isotropic homogeneous turbulence have been carried out. The simulations incorporate solutions for the marker field produced for a scalar having a simple source term proportional to the mean density. The mapping of the reaction progress field from this marker field is investigated at low to moderate Damkohler number and the results suggest that this could be a feasible way for closing the progress variable field in RANS and LES. Preliminary results for RANS calculations for a combustor with a backward-facing step are presented.

---

## 1. Introduction

Recently, methods of generating a simple marker field in turbulent premixed combustion have been proposed by Bilger (2004). In turbulent nonpremixed combustion, the mixture fraction has been a very powerful concept - its conservation equation is readily modeled and solved to give fields for its mean and variance in approaches involving Reynolds Averaged Navier Stokes (RANS) equations, see Bilger (1980) and Peters (2000). These fields provide a marker for the mixing, with reaction occurring near the instantaneous surfaces having the stoichiometric value of the mixture fraction. The progress variable,  $C$ , has been widely used in studies of turbulent premixed combustion (Peters 2000). While conceptually an ideal marker in turbulent premixed combustion, equations for its mean and variance have proved difficult to model satisfactorily in RANS and in Large Eddy Simulation (LES); it has the difficulty that its filtered values tend to be zero or unity everywhere in the flow except for a single surface of grid cells.

The new marker field,  $S$ , obeys the simple conservation equation Bilger (2004)

$$\rho \frac{\partial S}{\partial t} + \rho \mathbf{U} \cdot \nabla S - \nabla \cdot (\rho D \nabla S) = \rho / \tau_S \quad (1.1)$$

where the constant time scale,  $\tau_S$ , may be arbitrarily chosen - it merely sets the scaling for  $S$ . Equations for the mean and variance of  $S$  are obtained for stationary flow as

$$\bar{\rho} \tilde{\mathbf{U}} \cdot \nabla \tilde{S} + \nabla \cdot \overline{\rho \mathbf{u} s} = \bar{\rho} / \tau_S \quad (1.2)$$

$$\bar{\rho} \tilde{\mathbf{U}} \cdot \nabla (\overline{s'^2}) + \nabla \cdot \overline{\rho \mathbf{u} s^2} + 2 \overline{\rho \mathbf{u} s} \cdot \nabla \tilde{S} = -2 \bar{\rho} \tilde{N}_s \quad (1.3)$$

where

$$\tilde{S} \equiv \overline{\rho S} / \bar{\rho}; S = \tilde{S} + s \quad (1.4)$$

† The University of Sydney

$$\tilde{s}' \equiv \left( \frac{\overline{\rho s^2}}{\bar{\rho}} \right)^{1/2} \quad (1.5)$$

$$N_s \equiv D \nabla S \cdot \nabla S; \tilde{N}_s \equiv \overline{\rho N_s} / \bar{\rho} \quad (1.6)$$

It may be noticed that there are no unclosed chemical source terms in Eqs. 1.2 and 1.3. It is expected that standard RANS closures for the turbulent fluxes and for the scalar dissipation will be satisfactory, but this needs to be investigated.

It is conjectured in Bilger (2004) that for a statistically stationary one-dimensional turbulent premixed flame in homogeneous isotropic turbulence that the  $C$  field will be able to be mapped non-linearly from the  $S$  field at low to moderate Damhohler Numbers (Da). This is investigated here using 3D Direct Numerical Simulations (DNS). The DNS is described in the next section. The mapping of the  $C$  and  $S$  fields is investigated in Section 3, including conditional moment closure for obtaining  $C$  statistics from the  $S$  statistics. Application of the approach to a premixed combustor with a backward facing step is described in Section 4.

## 2. Direct numerical simulations

Direct numerical simulations of one dimensional premixed flames are carried out. The fully compressible Navier-Stokes equations with single step chemistry are solved:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \quad (2.1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_i u_j) = - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \quad (2.2)$$

$$\frac{\partial \rho e}{\partial t} + \frac{\partial}{\partial x_j} [(\rho e + p) u_j] = \frac{\partial u_j \tau_{ij}}{\partial x_i} + \frac{\partial}{\partial x_i} (\lambda \frac{\partial T}{\partial x_i}) + Q \omega \quad (2.3)$$

$$\frac{\partial \rho Y_R}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j Y_R) = \frac{\partial}{\partial x_i} (\rho D \frac{\partial Y_R}{\partial x_i}) - \omega \quad (2.4)$$

where

$$\rho e = \frac{1}{2} \rho u_i u_i + \frac{p}{\gamma - 1} \quad (2.5)$$

$$\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right) \quad (2.6)$$

$$\omega = A \rho Y_R \exp\left(-\frac{T_a}{T}\right) \quad (2.7)$$

$p$  is pressure,  $e$  is the internal energy and  $Q$  is the heat of reaction per unit mass of fresh mixture.  $A$  is the pre-exponential factor.  $T_a$  is the activation temperature. The gas mixture is assumed to be a perfect gas with a specific heat ratio of  $\gamma=1.4$ .  $Y_R$  is the normalized mass fraction of the deficient reactant. The reaction progress variable is defined here as  $C \equiv 1 - Y_R$ . The thermal conductivity,  $\lambda$ , and the diffusion coefficient,

---

Case	$u'/s_L$	$l_t/l_F$	$\rho_u/\rho_b$	$T_a/T_b$	Da	$Re_\lambda$
I	16.7	0.87	4	4	0.05	47
II	12.9	1.23	4	4	0.1	47
III	6.8	2.29	4	4	0.34	47

---

TABLE 1. Characteristics of the premixed flames

$D$ , are given as

$$\lambda = \mu c_p / Pr \text{ and } D = \mu / (\rho Sc) \quad (2.8)$$

The viscosity,  $\mu$ , is given as

$$\mu = \mu_u (T/T_u)^{0.76} \quad (2.9)$$

The Prandtl number,  $Pr$ , and the Schmidt number,  $Sc$ , are set to be 0.7. This formulation corresponds to a very lean fuel-air mixture (Trouve & Poinsot 1994).

The computation domain is a cube with inflow and outflow in the  $x_1$  direction and periodic in the  $x_2$  and  $x_3$  directions. The equations are integrated using a low storage fourth order Runge Kutta method with a sixth order compact finite difference scheme for spatial discretization (Kennedy *et al.* 2000; Lele 1992). A nonreflecting boundary condition is used for the outflow boundary (Poinsot & Lele 1992). The equations are solved on a  $178 \times 128 \times 128$  grid. Initial and inflow turbulence is homogeneous and isotropic. The characteristics of the premixed flames are shown in Table 1. The laminar flame thickness,  $l_F$ , is based on the maximum gradient of the progress variable. The results in Figs. 1-5 are those at  $\tau \approx 1.5$ , where the nondimensional time,  $\tau$ , is normalized by the initial eddy turn over time of the fresh mixture.

### 3. Mapping of the $C$ and $S$ fields

The conditional average of the reaction progress variable can be defined as

$$Q(\mathbf{x}, t, \varphi) \equiv \langle C(\mathbf{x}, t) | S(\mathbf{x}, t) = \varphi \rangle \quad (3.1)$$

where  $\varphi$  is the sample space variable of the marker,  $S$ . When the  $C$  and  $S$  fields are well correlated, the conditional fluctuations,  $c \equiv C - Q$ , will be small enough for the conditional moment closure (CMC) model to be applied for the closure of the nonlinear chemical reaction rate. Once the solution for  $Q$  is obtained, the statistics of  $C$  can be deduced from those of  $S$ , e.g.,

$$\tilde{C} = \int \tilde{P}(\varphi) \langle C | \varphi \rangle d\varphi \quad (3.2)$$

where  $\tilde{P}(\varphi)$  is the Favre probability density function (PDF) of  $S$ . In this section the mapping of the  $C$  and  $S$  fields will be investigated using the 3D DNS data. Figure 1 shows the conditional average,  $Q$ , and r.m.s. fluctuations,  $\langle c^2 | \varphi \rangle^{1/2}$ , for Case I. The maximum  $\langle c^2 | \varphi \rangle^{1/2}$  is about 0.08, which occurs at  $\varphi \approx 1.6$ . Figure 2 shows spatial distributions of  $C$  and  $S$  for Case I. The contour steps in  $S$  are uniform, while those in  $C$  are taken from the corresponding conditional average,  $Q$ , in Fig. 1. Note the strong similarity between the  $C$  and  $S$  fields mapped in this way.

The  $Q$  equation (derived below) involves the conditionally averaged reaction rate of

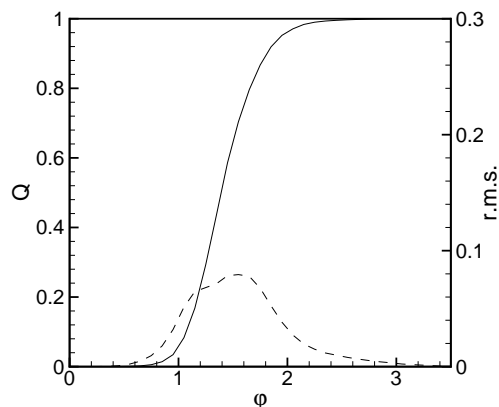


FIGURE 1. Conditional average and r.m.s. fluctuations of the reaction progress variable for Case I.

the progress variable,  $C$ . Conditional averaging suppresses fluctuations of reactive scalars when a proper conditioning variable is chosen. In the CMC model the nonlinear chemical reaction rates are closed using the conditional moments. First-order closure estimates of the conditional mean reaction rate in the conditionally averaged equation for the reaction progress variable using the conditional averages of reactive scalars:

$$\langle \omega(\rho, Y_R, T) | \varphi \rangle = \omega(\rho_\varphi, \langle Y_R | \varphi \rangle, \langle T | \varphi \rangle) = \omega(Q) \quad (3.3)$$

This closure is limited to 1-step chemistry. The closure model of Eq. (3.3) is tested in Fig. 3 giving excellent results for low  $Da$ .

Figure 4 shows the conditional average,  $Q$ , and r.m.s. fluctuations,  $\langle c^2 | \varphi \rangle^{1/2}$ , for higher  $Da$  cases, Cases II and III. As  $Da$  increases the slope of  $Q$  with respect to  $S$  increases so that the flame is in a narrower region of  $\varphi$  space. Also, the r.m.s.,  $\langle c^2 | \varphi \rangle^{1/2}$ , increases with  $Da$  so that the mapping between the  $C$  and  $S$  fields is not as good. This can also be seen from the contour plots in Fig. 5. The structures of the  $C$  and  $S$  fields are still similar for Case II. For Case III, however, the similarity between the  $S$  and  $C$  fields is not as good as in the lower  $Da$  cases, while the  $S$  and  $C$  fields are likely to have similar large scale wrinkling.

Figure 6 shows the conditional mean reaction rates for Cases II and III. The CMC closure for the reaction rate remains quite good, while the correlation between the  $C$  and  $S$  fields is not as good. It is not as good as at lower  $Da$ , but may still be sufficiently good for modelling purposes.

Next the  $Q$  equation is derived following Bilger (2004). Using the decomposition method described in Klimenko & Bilger (1999) the progress variable is split into a conditioned average and fluctuating component.

$$C(x, t) = Q(S(x, t), x, t) + c(x, t) \quad (3.4)$$

Derivatives are taken of this equation with respect to time and space and substituted into the conservation equation for the progress variable (given below), which after rearranging

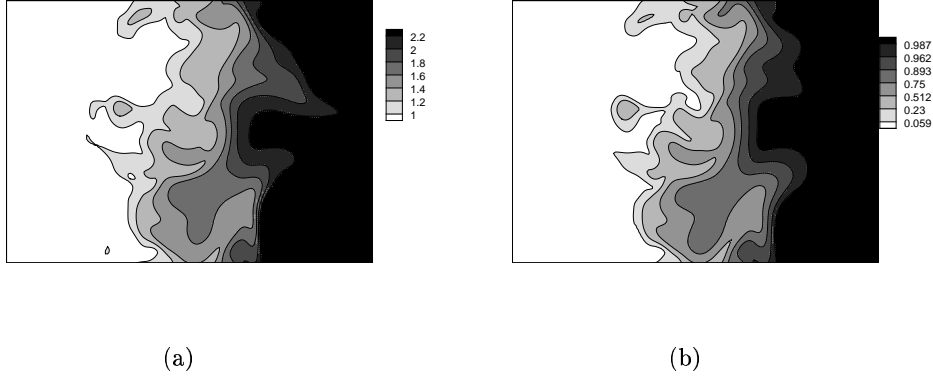
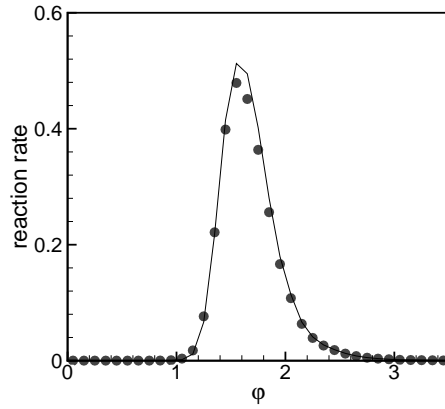
FIGURE 2. Distributions of  $C$  and  $S$  in a  $x_1$ - $x_3$  plane for Case I (a)  $S$  (b)  $C$ 

FIGURE 3. Conditional mean reaction rates for Case I(symbol: DNS, line: CMC).

gives

$$\begin{aligned} \rho \dot{Q} + \rho \mathbf{U} \cdot \nabla Q - \rho N_s Q'' + \left[ \rho \frac{\partial S}{\partial t} + \rho \mathbf{U} \cdot \nabla S - \nabla \cdot (\rho D \nabla S) \right] Q' = \\ \rho W_c / \tau_c - \rho \frac{\partial c}{\partial t} - \rho \mathbf{U} \cdot \nabla c + \nabla \cdot (\rho D \nabla c) \end{aligned} \quad (3.5)$$

$N_s = D \nabla S \cdot \nabla S$  is the scalar dissipation rate of  $S$ . Here the  $Q'$  signifies a derivative with respect to  $S$ . The fourth term on the LHS of Eq. 3.5 is simplified using Eq. 1.1 and the entire equation is divided by the density to give

$$\dot{Q} + \mathbf{U} \cdot \nabla Q - N_s Q'' + [1/\tau_s] Q' = W_c / \tau_c - \frac{\partial c}{\partial t} - \mathbf{U} \cdot \nabla c + \nabla \cdot (\rho D \nabla c) / \rho \quad (3.6)$$

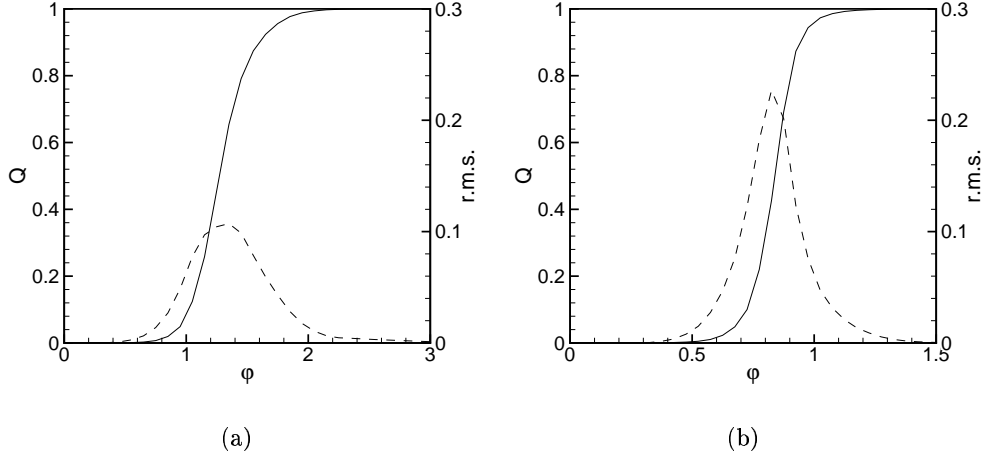


FIGURE 4. Conditional average and r.m.s. fluctuations of the reaction progress variable (a) Case II (b) Case III.

The equation is conditionally averaged following Bilger (2004) to give

$$\dot{Q} + \langle \mathbf{U} | \varphi \rangle \cdot \nabla Q - \langle N_s | \varphi \rangle Q'' + Q' / \tau_s = \langle W_c | \varphi \rangle / \tau_c + e_c \quad (3.7)$$

$$e_c = \left\langle -\frac{\partial c}{\partial t} - \mathbf{U} \cdot \nabla c + \nabla \cdot (\rho D \nabla c) / \rho | \varphi \right\rangle \quad (3.8)$$

The boundary conditions are  $Q = 0$  at  $S = -\infty$  and  $Q = 1$  at  $S = \infty$ . To make the solution more tractable several simplifying assumptions are made. First only steady state problems are addressed, so the time derivatives drop out. Based on a first order closure it is assumed that the first and third  $e_c$  terms are negligible. The reaction rate term is closed using Eq. 3.3. The  $S$  time scale is closed by  $\tau_s = L/U_u$ , where  $L$  and  $U_u$  are the inlet characteristic length and velocity, respectively. For 2D flow Eqs. 3.7 and 3.8 become

$$\langle u | \varphi \rangle \cdot \frac{\partial Q}{\partial x} + \langle v | \varphi \rangle \cdot \frac{\partial Q}{\partial y} - \langle N_s | \varphi \rangle Q'' + U_u / L Q' = W_c(Q) / \tau_c - \frac{\nabla [P(\varphi) \langle uc | \varphi \rangle]}{P(\varphi)} \quad (3.9)$$

A model is required to close the conditional velocity terms. Next the premixed CMC is derived and solved with Eq. 1.2 and 1.3 in a RANS model to show how  $C$  and  $S$  are related when Reynolds averaged. Solving Eq. 3.9 is left to future work.

#### 4. RANS application to a combustor

The premixed CMC method was originally proposed by Bilger (1993) and Smith (1994) and first implemented by Martin *et al.* (2003) and Martin (2003). The premise of the theory is that most of the fluctuations of the reactive scalars are correlated with a progress variable. The conservation equations for the species and energy are derived conditioned on the progress variable. This increases the dimensionality of the problem by one, while providing an improved closure for the reaction rates over other methods.

Next an outline of the derivation and the closure assumptions are given, followed by

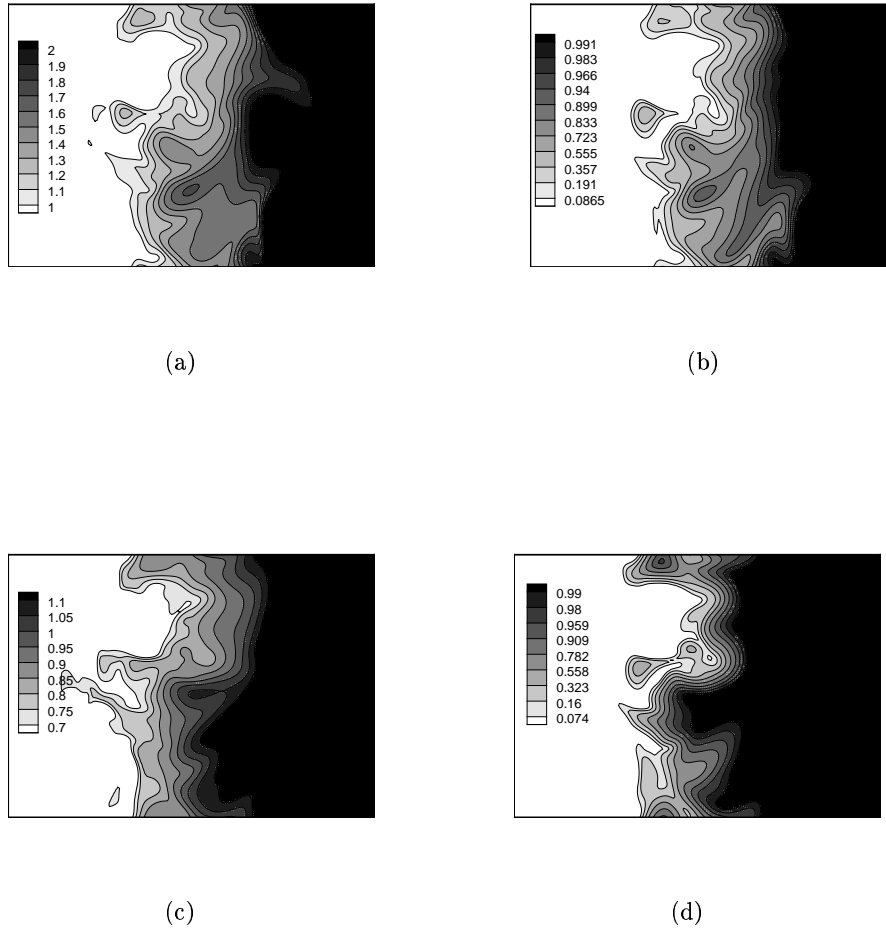


FIGURE 5. Distributions of  $C$  and  $S$  in a  $x_1$ - $x_3$  plane (a)  $S$  for Case II (b)  $C$  for Case II (c)  $S$  for Case III (d)  $C$  for Case III

the marker field implementation for RANS. Results are presented and future work is discussed.

#### 4.1. Derivation of the Premixed CMC Method

The premixed CMC method can be derived by two methods, following the non-premixed CMC. The first is the joint PDF method of Klimenko and the second is the decomposition method of Bilger, see Klimenko & Bilger (1999) for the details of the non-premixed derivations. Here the decomposition method is used. See Martin (2003) for a detailed derivation of both methods.

The derivation starts with the Favre averaged conditional expectation of the reactive

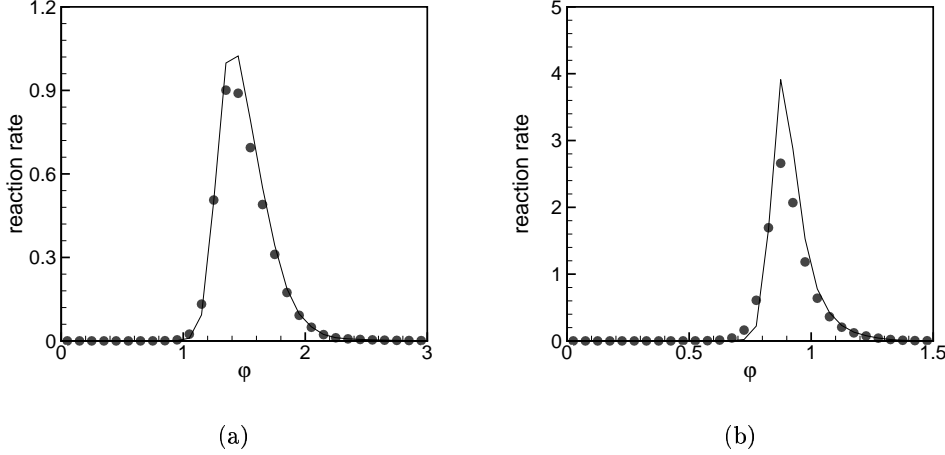


FIGURE 6. Conditional mean reaction rates (a) Case II (b) Case III (symbol: DNS, line: CMC).

scalar defined as

$$Q_i(\zeta, x, t) \equiv \frac{\langle \rho(x, t) Y_i(x, t) | C(x, t) = \zeta \rangle}{\langle \rho(x, t) | C(x, t) = \zeta \rangle} \quad (4.1)$$

Here  $Y$  is the species mass fraction and  $\zeta$  is the sample space variable corresponding to the progress variable  $C$ . The mass fractions are made up of the conditional averaged component and the fluctuation about this averaged value, shown below.

$$Y_i(x, t) = Q_i(C(x, t), x, t) + y_i(x, t) \quad (4.2)$$

This equation is substituted into the conservation equation for the species mass fractions shown below.

$$\rho \frac{\partial Y_i}{\partial t} + \rho \mathbf{U} \cdot \nabla Y_i - \nabla \cdot (\rho D \nabla Y_i) = \rho \omega_i \quad (4.3)$$

After simplification and employing the conservation equation for the progress variable the premixed CMC equation is obtained, shown below.

$$\langle \rho | \zeta \rangle \dot{Q}_i + \langle \rho u | \zeta \rangle \cdot \nabla Q_i = \langle \rho \omega_i | \zeta \rangle + \langle \rho D_i \nabla C \cdot \nabla C | \zeta \rangle Q_i'' - \langle \rho S_c | \zeta \rangle Q_i' + e_Q + e_y \quad (4.4)$$

$$e_Q = \langle [\nabla \cdot (\rho D_i \nabla Q_i) + \rho D_i \nabla C \cdot \nabla Q_i' + Q_i' \nabla \cdot (\rho (D_i - D_h) \nabla C)] | \zeta \rangle \quad (4.5)$$

$$e_y = -\langle [\rho \frac{\partial y_i}{\partial t} + \rho u \cdot \nabla y_i - \nabla \cdot (\rho D_i \nabla y_i)] | \zeta \rangle \quad (4.6)$$

$$\rho S_c = \frac{-\rho \sum \omega_i h_{f,i}}{h_{ad}^s - h_u^s} \quad (4.7)$$

Here the gradient operator signifies derivatives in real space, the primes indicate derivatives in  $C$  space and the dot indicates a time derivative. Note that  $S_c$  used here is the source term for the equation and is not the  $S$  from the marker field used above. Equation 4.4 is similar in form to the non-premixed CMC equation, with the third term on the



RHS of the equation the main difference. This term comes from  $C$  being a non-conserved scalar and can be thought of as a convective velocity in  $C$  space. This term makes the premixed equations stiffer than their non-premixed counterparts. In Eq. 4.7  $h_{f,i}$  is the heat of formation for the  $i$ th species and  $h^s$  is the sensible enthalpy. The ad subscript signifies adiabatic equilibrium conditions and the u indicates unburned conditions. Eq. 4.4 is in non-conserved form, the conserved form is obtained from the joint PDF derivation. The transport equation for the PDF of  $C$  can be used to convert between the two formulations.

To make the above equations more tractable several simplifying assumptions are made. The first is to assume steady state, so the time derivative terms drop out. The next assumption is that the conditioned mass fractions are constant in physical space, this eliminates the second term on the RHS of Eq. 4.4. This avoids the need for a closure model for the conditioned velocity. It is assumed that all diffusivities are constant and equal. The remaining terms in Eqs. 4.5 and 4.6 are assumed to be negligible for high Re flows. Klimenko & Bilger (1999) and Martin (2003) give a more detailed discussion on the magnitude of these terms. This gives the simplified premixed CMC equation as

$$\langle \rho D \nabla C \cdot \nabla C | \zeta \rangle Q_i'' - \langle \rho S_c | \zeta \rangle Q_i' + \langle \rho \omega_i | \zeta \rangle = 0 \quad (4.8)$$

This equation is decoupled from the flow field equations, with the conditioned scalar dissipation rate,  $\rho N_c = \langle \rho D \nabla C \cdot \nabla C | \zeta \rangle$ , the only value needed from the flow field (the dimensionality of the equations are reduced). This allows the simplified premixed CMC equations to be solved offline and saved in tabular format, greatly reducing the computation time. This is a system of  $ns+1$  equations, where  $ns$  is the number of species in the system, the extra equation is for the enthalpy. The equations reduce to a set of second order ODE's of the boundary value type, with the values at  $C = 0$  set to the unburned values and at  $C = 1$  set to the adiabatic equilibrium values. For adiabatic problems the enthalpy equation is not required.

#### 4.2. Closure Assumptions for RANS

The progress variable,  $C$ , is defined as the non-dimensional sensible enthalpy.

$$C \equiv \frac{h^s - h_u^s}{h_{ad}^s - h_u^s} \quad (4.9)$$

Using the sensible enthalpy instead of the temperature accounts for non-constant specific heats. The conservation equation for the Favre averaged  $C$  comes from the energy equation and the above definition.

$$\frac{\partial \bar{\rho} \tilde{C}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{\mathbf{U}} \tilde{C}) - \nabla \cdot (\mu_t / \sigma_c \nabla \tilde{C}) = \bar{\rho} \tilde{S}_c \quad (4.10)$$

$\sigma_c = 0.7$ , is the turbulent Schmidt number.  $S_c$  is the conditioned source term as defined in Eq. 4.7. Similarly the conservation equation for the variance of the progress variable is derived.

$$\frac{\partial \bar{\rho} \tilde{c}^2}{\partial t} + \nabla \cdot \bar{\rho} \tilde{\mathbf{U}} \tilde{c}^2 - \nabla \cdot (\mu_t / \sigma_c \nabla \tilde{c}^2) = C_{c1} \mu_t (\nabla \tilde{C})^2 - C_{c2} \bar{\rho} \frac{\tilde{\epsilon}}{k} \tilde{c}^2 - 2 \bar{\rho} \tilde{S}_c'' \quad (4.11)$$

A closure for the fluctuation of the source term, the last term on the RHS of Eq. 4.11 is obtained by doing a Taylor series expansion, see Martin (2003) for the details.  $C_3 = 100$ ,

other values were tried with little affect on the solution.

$$\widetilde{S}_c' = C_3 \frac{\widetilde{c}^2}{\widetilde{T}(\widetilde{C} + \frac{\widetilde{T}_u}{T_{ad} - \widetilde{T}_u})} \widetilde{S}_c \quad (4.12)$$

The conditioned scalar dissipation is approximated by the unconditioned value as.

$$\langle \widetilde{N} | \zeta \rangle \simeq \widetilde{N} = 2 \frac{\widetilde{\epsilon}}{\widetilde{k}} \widetilde{c}^2 \quad (4.13)$$

The solution procedure is to solve the simplified premixed CMC equations for a range of scalar dissipation values and store the density, source term and species mass fractions in a table. Fluent ver. 6.1.22 (Fluent 2004) is used to solve the fluid equations along with the RNG turbulence model for the 2-dimensional backward facing step of El Bahawy *et al.* (1983). Premixed methane and air are flowed over the step and the flame is stabilized in the recirculation zone. The equivalence ratio is 0.9 and the full GRI2.11 mechanism is used (Bowman *et al.* 1998). An initial mesh of 300 x 80 cells is used with grid adaption in the flame zone and along the wall to meet the log-wall criteria for the wall boundary conditions. Equations for the progress variable and its variance are added as scalar equations to (Fluent 2004) using its user defined function (UDF) capabilities. The inlet values are zero and the outlet and walls are set to zero gradient for the scalars.

At each computational cell, the mean progress variable and scalar dissipation is used to retrieve the conditioned density, reaction rate source term and mass fractions from the table. The progress variable and its variance are used with an assumed shape beta-function PDF to obtain the non-conditioned values, which are used in the next iteration of the CFD code. This process is continued until steady state is reached.

#### 4.3. Marker Field Implimentation

Here a comparison is made between the  $C$  field using Eq. 4.8 and the  $S$  field, without using Eq. 3.9. Future work will calculate the  $C$  field using Eq. 3.9.

Equations 1.2 and 1.3 are also added to (Fluent 2004) as additional UDF's. The inlet values for  $S$  are  $-20(1 - y/h)$ , where  $y$  is the vertical coordinate of the step and  $h$  is the step height. Standard RANS closure is used for the turbulent fluxes. There is no feed back from the marker field equations to the other equations. The scalar dissipation of  $S$  is calculated as follows.

$$\langle \widetilde{N} | \zeta \rangle \simeq \widetilde{N} = 2 \frac{\widetilde{\epsilon}}{\widetilde{k}} \widetilde{s}^2 \quad (4.14)$$

#### 4.4. RANS Results

Figures 7 and 8 show the progress variable and its variance, showing the location of the flame front. Figure 9 shows the scalar dissipation of the progress variable. The large values in these figures at the tip of the step are due to limitations in the turbulence model and are not physical. Figure 10 shows the marker field. The contours in the flame zone are nearly parallel with the progress variable contours, indicating a potential mapping between the progress variable and the marker field. Figure 11 shows the variance of the marker field, which is very different then the variance of the progress variable. The variance of the marker variable was nearly zero until reaching its peak at the flame zone, then slowly tapering off. The variance of the marker field is largest prior to the flame and tappers off as the flame zone is approached. Figure 12 shows the scalar dissipation of the marker field. The peak values are in the flame zone, as was the case with the progress variable, but it also has large values prior to the flame zone.



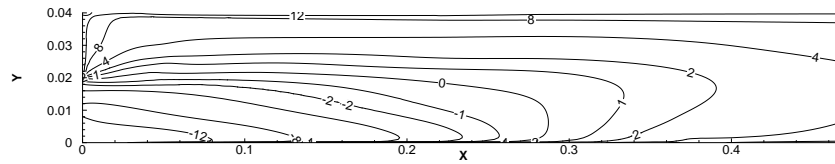
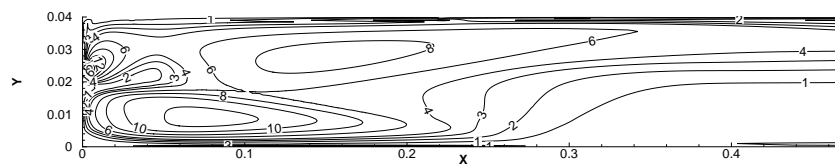
FIGURE 10. Marker variable,  $S$ .

FIGURE 11. Variance of marker variable.

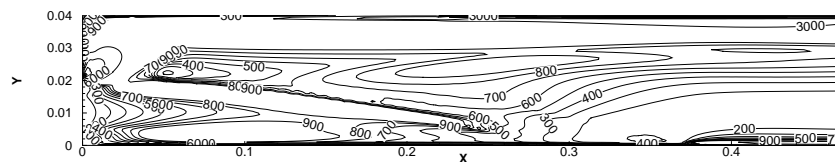


FIGURE 12. Marker variable scalar dissipation.

- BILGER, R. W. 1980 in *Turbulent Reacting Flows*, P.A. Libby and F.A. Williams, Eds., pp267-285 Elsevier Science Publishers.
- BOWMAN, C.T., HANSON, R.K., DAVIDSON, D.F., GARINER JR., W.C., LISSIANSKI, V., SMITH, G.P., GOLDEN, D.M., FRENKLACH, M. & GOLDENBERG, M. 1998 [www.me.berkeley.edu/gri-mech/GRI2.11](http://www.me.berkeley.edu/gri-mech/GRI2.11).
- EL BANHAWY, Y., SIVASEGARAM, S. & WHITELAW, L.H. 1983 Premixed, Turbulent Combustion of a Sudden-Expansion Flow. *Combust. Flame* **50**, 153-165.
- FLUENT CFD CODE, 2004 [www.fluent.com](http://www.fluent.com).
- KENNEDY, C. A., CARPENTER, M. H. & LEWIS, R. M. 2000 Low-storage, explicit Runge-Kutta schemes for the compressible Navier-Stokes equations. *Appl. Num. Math.* **35**, 177.
- KLIMENKO, A.Y. & BILGER, R. W. 1999 Conditional Moment Closure for Turbulent Combustion. *Prog. Eng. Comb. Sci.* **25**, 595-697.
- LELE, S. K. 1992 Compact finite difference schemes with spectral-like resolution. *J. Comp. Phys.* **103**, 16.
- MARTIN, S.M., KRAMLICH, J.C., KOSALY, G. & RILEY, J.J. 2003 The Premixed Conditional Moment Closure Method Applied to Idealized Lean Premixed Gas Turbine Combustors. *Journal of Engineering for Gas Turbines and Power, Transactions of the ASME* **125**, 895-900.

- MARTIN, S.M. 2003 *Ph.D Thesis, The Conditional Moment Closure Method for Modeling Lean Premixed Turbulent Combustion*. The University of Washington.
- PETERS, N. 2000 *Turbulent Combustion*. Cambridge University Press.
- POINSOT, T. J. & LELE, S. K. 1992 Boundary conditions for direct numerical simulations of compressible viscous flows. *J. Comp. Phys.* **101** 104.
- SMITH, N.S.A. 1994 *Ph.D Thesis, Development of the Conditional Moment Closure Method for Modelling Turbulent Combustion*. The University of Sydney.
- TROUVE, A. & POINSOT, T. 1994 The Evolution Equation for the Flame Surface Density in Turbulent Premixed Combustion. *J. Fluid Mech.* **278**, 1-31.