FLAME KERNEL INTERACTIONS IN A TURBULENT ENVIRONMENT

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Abstract. Results are presented from a parallel DNS combustion code called SENGA. The code solves a fully compressible reacting flow in three dimensions. High accuracy numerical schemes have been employed which are explicit 10th order central finite differences in space, a third order explicit Runge-Kutta method in time and parallel implementation is achieved through the Message Passing Interface (MPI). Turbulence is generated numerically for a 128^3 simulation with Re = 30 and a 384^3 simulation with Re = 130. Finally, results are presented and discussed for simulations with different initial non-dimensional turbulence intensities ranging from 5 to 23.

1. Introduction

A difficulty that arises in practical turbulent combustion processes, such as the combustor sections of jet engines and internal combustion engines, is the strong coupling between turbulence, chemical kinetics and heat release. These interactions are generally three dimensional and time dependent, and are not easily accessible to experimental investigation. Therefore, to extract valuable information from these and other turbulent flows, highly accurate numerical solutions are required, such as those obtained using Direct Numerical Simulation (DNS).
DNS is now a useful and well established research tool in the field of tur-

bulent combustion. The solution of the full governing equations without the need for any form of turbulence modelling enables the collection of a great deal of information on turbulent flame structure and propagation that is obtainable by no other means. However, to obtain representative simulations, the DNS must be able to resolve the smallest length and time scales applicable to the problem of interest. High resolution and the need to solve in three spatial directions and time comes at a cost, therefore parallel supercomputers are a pre-requisite to carry out these simulations. Due to the high computational costs, it is important to use high accuracy spatial discretisation schemes. The most accurate scheme is the Fourier spectral method, however, these schemes are restricted to problems with periodic boundary conditions which in combustion DNS is a restriction since reactants must be able to enter and products and heat must be able to leave the computational domain. Therefore alternative schemes with spectral like accuracy and non restrictive boundary conditions are required, the most popular scheme for combustion being the compact scheme (Lele, 1992). In the present work, 10th order explicit finite differences are employed. These offer near spectral accuracy along with inflowing and outflowing boundary conditions and are more efficient for parallel implementation. (Prosser and Cant, 1998) compared various spatial schemes applicable to combustion DNS, and showed the explicit scheme to perform well in terms of accuracy when the resolution is known to be sufficient, and in terms of CPU time and storage the explicit schemes proved least expensive on both counts.

Practical combustion problems have chemical and turbulent scales and in most cases it is the smallest chemical scales within the reaction zone of the flame that are of interest, not the smallest turbulent scales. This is true for example in the spark ignition engine where combustion takes place in a reasonably homogeneous mixture of fuel vapour and air, and where the turbulence is of moderate intensity. These kind of systems operate within the laminar flamelet regime of turbulent premixed combustion (Libby and Williams, 1994). Here the thickness of the flame sheet remains smaller than the Kolomogorov scale of turbulence and the Kilmov-Williams criteria is satisfied (Williams, 1985). The flame sheet retains the structure of a laminar flame, even though it is wrinkled by the surrounding turbulence. The flame-turbulence interactions in the present work are in the above regime and therefore the flame structure and not the turbulence defines the resolution requirement. Research in combustion DNS as come a long way in these regimes (Poinsot *et al.*, 1996), especially for planar flames. The present work uses flame kernels in a turbulent environment which have a practical relation to ignition problems. The growth of the flame is laminar once established in the early stages, and then propagates spherically outwards. Its motion is accelerated by flow divergence due to thermal expansion and it

begins to interact with the surrounding turbulence becoming wrinkled and increasing in surface area. Flame kernels in conjuction with non-reflecting outflow boundaries on all faces using the NSCBC formalism (Poinsot and Lele, 1992), allow the flame structure to be observed away from the influence of any boundary impositions.
The aim of the present research is to use a parallel DNS code called SENGA, developed in Cambridge, to study flame kernels in a turbulent environment. The DNS code solves the fully compressible reacting flow equations in three dimensions and time with heat release. The paper is organised as follows. The equations governing the flow are outlined in non-dimensional format, the numerical procedure is explained and finally the simulation method and results are presented for various flame turbulent interactions.

2. Governing Equations

The governing equations that describe the motion of a reacting gas are the three dimensional equations for mass, momentum, energy and a species conservation equation (Williams, 1985). In non-dimensional form these equations become.

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_k}{\partial x_k} = 0 \tag{1}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_k u_i}{\partial x_k} = -\frac{\partial P}{\partial x_k} + \frac{1}{Re}\frac{\partial \tau_{ki} u_i}{\partial x_k} \tag{2}$$

$$\begin{aligned} \frac{\partial \rho E}{\partial t} + \frac{\partial \rho u_k E}{\partial x_k} &= -(\gamma-1)\mathcal{M}^2 \frac{\partial P u_k}{\partial x_k} \\ &\quad + \frac{1}{Re}(\gamma-1)\mathcal{M}^2 \frac{\partial \tau_{ki} u_i}{\partial x_k} \\ &\quad + \frac{\tau}{RePr}\frac{\partial}{\partial x_k}(\lambda \frac{\partial T}{\partial x_k}) \\ &\quad - \frac{\tau}{ReSc}\frac{\partial}{\partial x_k}(\rho D \frac{\partial c}{\partial x_k}) \end{aligned} \tag{3}$$

$$\frac{\partial \rho c}{\partial t} + \frac{\partial \rho u_k c}{\partial x_k} = \omega_\alpha + \frac{1}{ReSc}\frac{\partial}{\partial x_k}(\rho D \frac{\partial c}{\partial x_k}) \tag{4}$$

where x and t are the space and time coordinates, ρ is the density, u is the velocity , P is the pressure, E is a stagnation internal energy, c is a reaction progress variable, formulated as a normalised mass fraction and rising monotonically from zero in the unburned state to unity in the fully burned products and τ_{ki} is the viscous stress tensor
The non-dimensional parameters in the above equations are the Mach num-

ber $\mathcal{M}$, the Reynolds Number Re, the Prandtl number Pr and the Schmidt number Sc. For a full description of the non-dimensionisation and the extra terms needed to close the problem, see (Jenkins and Cant, 1999).

3. Numerical Procedure

Turbulent combustion DNS requires spatial schemes with high accuracy. Therefore, all first and second spatial derivatives are discretised using a central 10^{th} order explicit scheme obtained from the central finite difference approximation

$$f_i' = \sum_{j=1}^{m/2} \frac{a_j}{2jh}(f_{i+j} - f_{i-j})$$

where m is the order of the approximation (always even). Values of constants a_j are obtained by expanding in Taylor series and equating coefficients of successive orders in h.

These finite difference approximations have a stencil width of eleven points which implies 5 points are required at the boundary. These boundary points are again treated with explicit finite differences of decreasing accuracy to the boundary. This is covered in detail by (Jenkins and Cant, 1999). Time stepping is carried out by an explicit third order Runge-Kutta method (Wray, 1990). This method requires three sub steps for each main time advancement step and requires only two storage locations, one for the time derivative and one for the dependent variable.

An initial field of isotropic turbulence is generated numerically to satisfy the continuity constraint for incompressible flow. The general requirement for this turbulent field is the specification of an energy spectrum E(k), where k is a wavenumber in the Fourier-space representation of the turbulent velocity field. Various energy specta exist for this work such as (Lee and Reynolds, 1985) which as previously been used by the authors. However, the present work uses the spectrum of (Schumann and Patterson, 1978) after studies showed a slower decay in turbulent kinetic energy compared to Lee and Reynolds. This is of interest, especially for higher turbulence intensity cases, were the flame interacts longer at the higher intensities. Finally, boundary conditions are implemented using the Navier Stokes Characteristic Boundary Conditions (NSCBC) (Poinsot and Lele, 1992) and parallel implementation is achieved through the Message Passing Interface (MPI).

4. Simulation Results

Flame kernel interactions for various turbulent intensities will be presented. Two simulations were undertaken, one with a grid size 384^3 and the other with a grid size 128^3. Both simulations were undertaken using 64 processors on the Hitachi SR2201 at Cambridge University and table 2 shows the problem parameters for each case.

TABLE 1. Simulation Parameters

Case	Re	Pr	Sc	M	β	α	τ	B
128^3	30	0.7	0.7	0.00142	6.0	5.0	0.83	1225.0
384^3	130	0.7	0.7	0.00142	6.0	5.0	0.83	1225.0

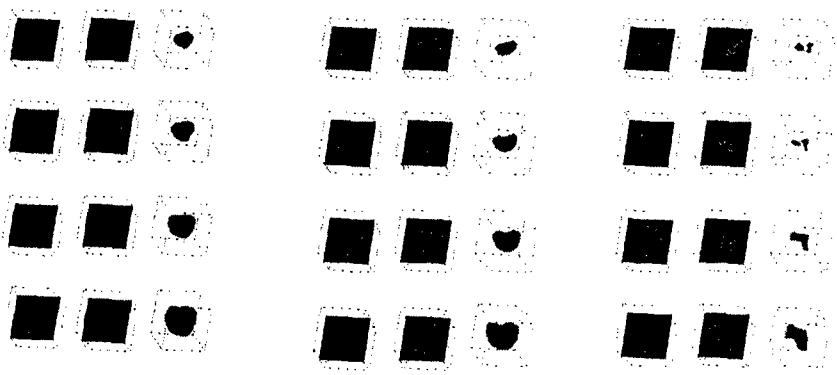
In both cases, the simulations were initialised by a Gaussian distribution of the progress variable c decomposed on the 64 processors with an initial turbulent field. All boundary conditions were non-reflecting outflow types with a time step $\Delta t = 1.0 \times 10^{-6}$ which is restricted by the acoustic Courant stability criteria. Initial studies on small grids (64^3) have been undertaken with $\mathcal{M} = 0.0142$, enabling larger time steps $\Delta t = 1.0 \times 10^{-4}$. Computational performance is reasonable, with the initial turbulent fields taking approximately 8 and 20 minutes to generate for 128^3 and 384^3 simulations respectively, and time stepping takes approximately 15 and 50 seconds for each case. A full parallel performance test can be found in (Jenkins and Cant, 1999).

Figures 1a - 1c show results from initial $\frac{u'}{S_L}$ values of 5, 10 and 23 respectively. In each figure, three sets of results are plotted at 2, 4, 6 and 8 thousand time steps. The left and centre columns show a 2D slice from a laminar and turbulent flame and the right column shows the isosurface of progress variable c, all at the same time levels respectively. The laminar and turbulent flame cases are plotted with progress variable contours ranging from 1 (fully burned) at the centre to 0 (unburned) on the outer contour. In each case the flames can clearly be seen to propagate outwards. As the flames develop the effect of turbulence on them becomes less significant, since the turbulence is decaying. From these figures, an important feature of the flame is clear. Small scale wrinkles in the flame, more noticeable at $\frac{u'}{S_L}$ =23, do not remain. They appear to be smoothed out as the flame propagates. Also evident at high turbulence intensity is the flame breaking up and re-joining as the turbulence decays.

Figures 2a and 2b show a (128^3) flame evolution at the centre x-y plane

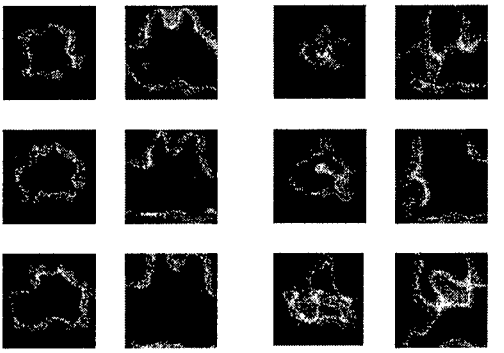
(k=64) and the quarter x-y plane (k=96) over time starting at the top left and going to the bottom right of each figure. Two interesting features occur in these figures, the first being an increase in burned area with time about the initial ignition point and the second is the evidence of holes in the flame due to strain. The holes are more noticeable in figure 2b. Here the image plane is initially at the edge of the flame and as the flame progresses holes and break up are evident. Figure 3 looks at an enlarged portion of the centre plane. Here the flame front is moving to the right and upwards. Velocity vectors are superimposed on to the flame contours to show the effect of flame curvature due to the eddies in the turbulent field. Also at the points of maximum curvature the flame thickness seems to be increasing due to a higher burning rate, since the surface area is increasing.
Finally, figure 4 shows an isosurface of the progress variable at c = 0.8. The image shown is for the inner 8 processors of a 64 processor simulation. This is evident by the rings on each surface due to the flame leaving one processor and joining the next. This is a good indication of the velocity of the parallel implementation as well as visualising in three dimensions the flame surface.

5. Figures



(a) $\frac{u'}{S_L}$=5 (b) $\frac{u'}{S_L}$=10 (c) $\frac{u'}{S_L}$=23

Figure 1. laminar, turbulent and isosurfaces for 3 turbulent cases t = 2k - 8k



(a) Centre Plane (b) Quarter Plane

Figure 2. 2D slice at centre x-y plane and quarter x-y plane

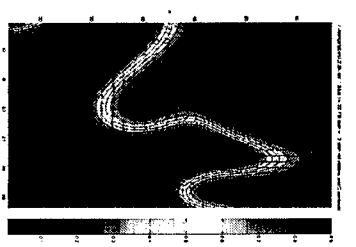


Figure 3. Enlarged 2D slice of progress variable contours and velocity vectors

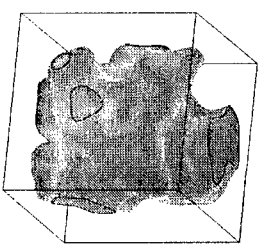


Figure 4. Isosurface of progress variable, c = 0.8

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