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Visualisation of Results from LES of Combustion

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***Abstract*:** We examine the role of visualisation in the context of LES simulations of premixed turbulent combustion. The physical processes involved in premixed turbulent combustion are extremely complex, and the modelling of both the turbulence (via LES) and the combustion (via flame-wrinkling models) is difficult. Appropriate visualisation is required to understand the behaviour of the models, and ultimately to understand better the flow processes which are important in many industrial applications. We examine visualisations of two specific cases; simple flame kernel growth in a box of turbulence, and combustion behind a backward-facing step. A number of visualisation techniques are used to produce results that are similar to experimentally determined Schlieren and Mie photography for the flame kernel. In addition, isosurfaces of the reaction regress variable coloured by the laminar flame speed and sub-grid wrinkling are also plotted in an attempt to gain deeper insight into the physics of turbulent combustion in the context of these particular cases. Finally we discuss the role of the WWW in the continuing development of scientific visualisation techniques.

***Keywords*:** large eddy simulation, combustion, Schlieren, computer simulation.

1. Introduction

Although the governing equations of fluid dynamics, the Navier-Stokes equations (NSE) have been known for more than 150 years, they are strongly non-linear, and so typically cannot be solved analytically. The increasing power of computers provides an alternative, however, the numerical solution of the equations, often coupled with modelling of the physics. This is known as Computational Fluid Dynamics, or CFD. This can be used to supplement experimental investigation, easily providing data about the flow which it is difficult to measure, and thus contributing to the understanding of the flow. CFD can be used in two ways, to provide quantitative results for particular cases (such as the lift force on an aerofoil of specific geometry), and to provide a qualitative understanding of the flow patterns and physics of a particular case. Although the first might generate specific numbers, such as lift and drag coefficients, the second requires visualisation of the results — in fact, given the vast amounts of data generated from a typical simulation, much care and thought has to be put into visualising the data in the best possible way. An improved understanding of the flow from such a visualisation can help in the design process, particularly as it is relatively easy to change the geometry and repeat the calculation to see what difference design changes make. For this reason, CFD is making increasing inroads in industry, and changing the nature of the design process in any engineering situation involving fluids.

This paper concentrates on the visualisation of simulations of premixed turbulent combustion. Turbulence is a complex flow regime, characterised by the existance in the flow of pseudo-random eddies at scales ranging from large eddies, whose scale is determined by the geometry, down to small eddies at scales fixed by the viscosity of the fluid. Energy enters at the largest scales, and cascades downwards by a process of interactions between eddies, eventually being dissipated by viscous processes at the smallest scales. Full solution of the NSE for such a system is possible — known as DNS — but only for relatively simple geometries without additional physics being included. More commonly, some sort of filtering is first applied to the NSE to produce equations describing the mean flow. This leaves a random 'turbulent' component to the motion, which has to be modelled in some way. The addition of further complex physics complicates matters still further. In the case of combustion, the heat release and change of properties associated with the combustion modifies the flow significantly (the coupling is in both directions, with the rate of combustion being influenced by the flow as well). In premixed combustion, the fuel and oxidant are already mixed together at the molecular level; when ignited a flame front propagates through the mixture, leaving reacted products behind. Such combustion is typical of internal combustion engines, for example, and its study is therefore of prime industrial importance. Over the years we have developed models of premixed turbulent combustion using a turbulence modelling technique called Large Eddy Simulation (LES). Our interest here is to visualise the results, to better understand the physics involved (and hence improve the model) as well as to be able eventually to contribute to the design of devices involving premixed turbulent combustion.

The use of visualisation has been an important aspect of DNS and LES of turbulent flow from the landmark results of Moin and Kim in the early 80s [Moin and Kim:1982]. They produced a video showing the trajectories of marker particles for channel flow which they state was one of the best received aspects of their work within the turbulence community. Since that time visualisation in DNS and LES has used similar techniques to other areas of unsteady CFD. For instance, Freitas [1991] has used an 'advanced flow visualisation system' to post-process velocity and temperature field results from the DNS of natural convection within a finite enclosure. A large body of work exists (e.g. [Jeong and Hussain:1995]) on the eduction of vortex structures which are responsible for a large percentage of the momentum and species transport within turbulent flows, but the actual methods used to visualise these structures once they are found are on the whole fairly straightforward. Where combustion takes place visualisation of some quantity giving the degree of reactedness has often been used (e.g. the reaction progress variable for premixed combustion [Kim et al.: 1998] and the mixture fraction in non-premixed combustion [Luo:1997]) to give an indication of the instantaneous position of the flame surface.

2. LES and Combustion Modelling

In order to simplify the mathematical system describing a turbulent flow, elements of the system must be removed by filtering and subsequently modelled. In LES the filtering is done in terms of spatial scales: a filter function is specified (typically a top hat function in real space) and convolved with the NSE. The result is a filtered set of equations describing the dynamics of those eddies which are larger than the filter width. These large eddies will be affected by the geometry of the case (e.g. will be constrained by walls) and thus will need to be explicitly calculated. Eddies smaller than the filter will not be so affected, and will be similar in all parts of the flow domain and at all times. They can thus be replaced by a simplified model. The filtering process has removed them from the equation of motion, their effect on the large scales being replaced by the new terms in the equations. LES modelling consists of finding models for these terms in terms of subgrid-scale properties, so-called because typically the computational mesh used for the calculation sets the filter scale. Here we use a model for the SGS turbulent kinetic energy k derived using the Boussinesq approximation, known as the 1-Equation Eddy Viscosity model [Fureby et al.:1997].

For the combustion modelling, we use a family of models developed in our group [Weller et al.:1994; Weller:1993; Weller et al.:1998]. These are known as flame wrinkling models. In a laminar (non-turbulent) flow a flame front will propagate at a fixed speed determined by the physics of the gas and its chemical properties. In a turbulent flow, the flame front will propagate in this manner at the smallest scales: at larger scales it will become wrinkled, and this wrinkling will enhance the propagation speed of the whole front. LES filtering creates a mean flame front which will propagate at this enhanced speed. An indicator function b can be introduced which takes values 1 in the unburnt gas and 0 in the burnt gas, and the location of the mean flame front is given by the variation of the filtered value, $\overline{b}$, between these values. Its velocity is a function of the gradient $\nabla\overline{b}$, of mean strain in the flow, of the laminar flame speed S_0, and of the subgrid-scale wrinkling. This is expressed in terms of a wrinkling parameter Ξ (defined as the ratio of the total flame area to the projected flame area), for which we produce various models. Thus to understand the behaviour of the model we need to look at all of these effects.

Having set up the mathematical equations describing the modelled system, the next step is to solve them. For this we make use of the Finite Volume (FV) method; the computational domain V is divided into a collection of cells or control volumes δV_i which pack V, i.e., $V=\sum i \delta V_i$. The transport equations are integrated over each control volume, and Gauss' theorem used to turn the equations into a set of linked difference equations which can be solved numerically. A research code written in C++, FOAM [Weller et al.:1998b], is used for this purpose. The advantages of the FV formulation are that it is intuitive, easy to link to the physical situation, and since the control volumes can be of any shape, can be applied to any geometry with any topology desired. The resulting output is field data consisting of scalar, vector or tensor data corresponding to each control volume in the domain. It is then the task of visualisation to display this data in a convenient manner for the user to interpret. We use two visualisation packages. One is the commercial product AVS Express, whilst the other is a shareware product produced by a group in GE, VTK.

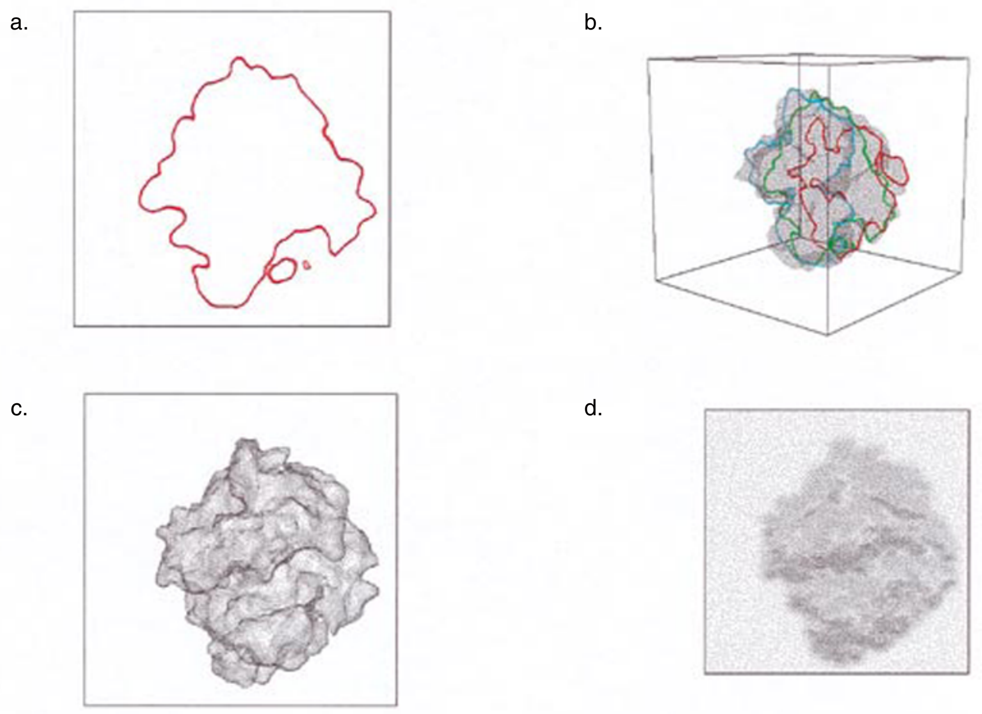

Fig. 1.

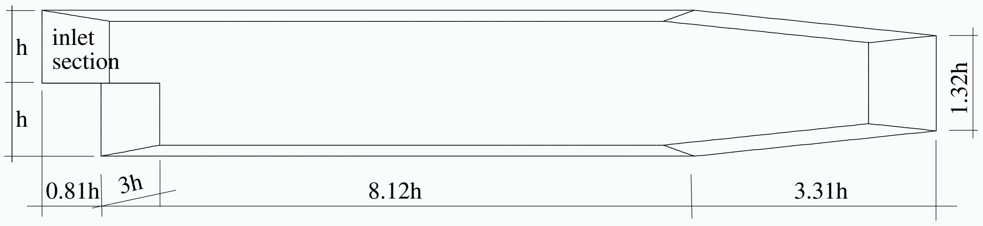

Fig. 2.

3. Comparison with Experimental Visualisation

We discuss two test cases in this paper, being combustion in isotropic homogeneous turbulence (a bomb combustor), and combustion behind a backward-facing step. In this section techniques to compare with experimental visualisation are discussed with reference to the bomb combustor. In the next section, visualisation techniques used to gain greater physical insight are discussed, and the backward-facing step is introduced.

A bomb combustor is an enclosed chamber in which premixed fuel and oxidant can be ignited. This is a popular experimental setup, since the various parameters can be readilly controlled. Unpublished experimental data from work carried out at Leeds University, U.K. is used here in which turbulence levels are controlled by 4 fans arranged tetrahedronally, and the mixture is ignited by a spark plug, leading to a roughly spherical flame front (the kernel) which expands through the domain. Windows in the bomb permit optical access for measurement and recording. The results shown are for premixed iso-octane and air at an equivalence ratio of 1.0. The initial pressure and temperature are 1 atmosphere and 358K respectively while the turbulence intensity is 2.36m/s and the integral length scale is approximately 20mm. The unstrained laminar flame speed is 0.434m/s. A good approximation to this case is that of a cubic box domain with cyclic boundary conditions (which is the computational equivalent of an infinite homogeneous and isotropic domain) which is forced to remain turbulent by large-scale stochastic forcing. Ignition is achieved by burning a number of cells at the centre of the domain over a finite time, and the temporal evolution of the kernel simulated. A box with $64^3 = 262144$ cells was utilised for this purpose.

Here we discuss two methods for experimentally visualising the flame surface, via Schlieren and Mie photography. In Mie scattering (or laser sheet tomography) the unburnt flow is seeded with, for instance, silicone oil droplets that evaporate upon crossing the flame front. A laser sheet is then produced using a combination of spherical and cylindrical lenses and the difference in the optical scattering properties of the liquid droplets and the vapour gives an indication of the instantaneous flame position which may be extracted using edge detection algorithms. This may be easily simulated by plotting contours of $\overline{b}$ on planes intersecting the kernel. See Fig. 1a. The problem with this technique is that the kernel can move quite substantially due to large-scale turbulent velocity fluctuations in the experiment, so it is not easy to ensure that the laser sheet bisects the kernel, or in fact intersects it at all. Multiple intersections of the plane of the laser sheet are possible Fig. 1a. This may give the impression that the flame surface actually consists of multiple topologically distinct regions. Examining the transparent isosurface in Fig. 1c. this can be seen not to be the case. To further illustrate this point Fig. 1b. shows the two dimensional flame countour at three possible locations on a partially transparent flame kernel illustrating how care must be taken in interpreting the results.

In Schlieren photography, light rays passing through the experimental apparatus are focussed onto a mask of some kind (typically a knife edge), and the resulting masked pattern is imaged with a second lens. If the light paths through the apparatus are disturbed by gradients in the refractive index normal to the direction of propagation, this will shift the transform image at the knife-edge, and brightening or darkening the image relative to a non-affected path. The technique thus images gradients in the refractive index normal to the direction of viewing. These

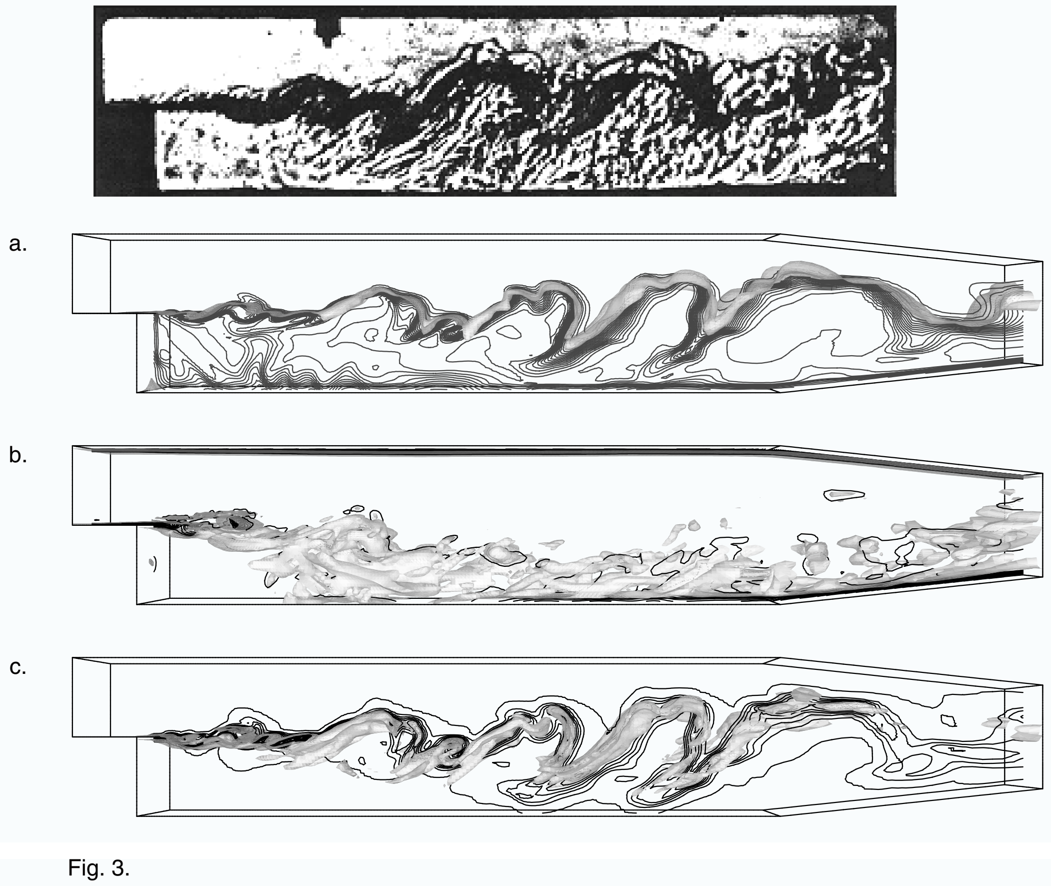

Fig. 3.

gradients are representative of the temperature distribution, i.e. the flame surface. Thus a simplified way of visualising the computational results is to project a partially transparent isosurface of $\overline{b}$ onto the back plane. This can be done using an orthographic projection, and produces the view shown in Fig. 1c. However using volume rendering techniques, a more physically accurate visualisation can be constructed. Knife-edge Schlieren visualises temperature gradients in a given direction, $\nabla T \cdot \mathrm{n}$, which can easilly be constructed from the data. The value and sign of this quantity can be used to control the colour (from black to white) and opacity (a saw-tooth function, with undeviated rays being almost transparent, and greater values of $|\nabla T \cdot \mathrm{n}|$ being more opaque) in the volume renderer. The results are shown in Fig. 1d. Other types of Schlieren photography such as aperture-based photography could also be simulated in this way, as could shadowgraph photography, in which the second derivative of T is being visualised.

4. Visualisation of the Physics

The second case is that of combustion behind a backward-facing step. Figure 2 shows the geometry, in which premixed fuel and air from the inlet at the left pass over the step. The mixture is ignited and a flame front forms in the region of the shear layer. Because of its location the behaviour of this flame front is extremely complex and its prediction very difficult. Large eddy simulations have been carried out of an earlier experiment [Pitz and Daily:1983]. The mixture consists of premixed propane and air at an equivalence ratio of 0.57. The inlet velocity is 15.3 m/s and the ambient pressure and temperature are 1 atmosphere and 293K. The computational grid consists of

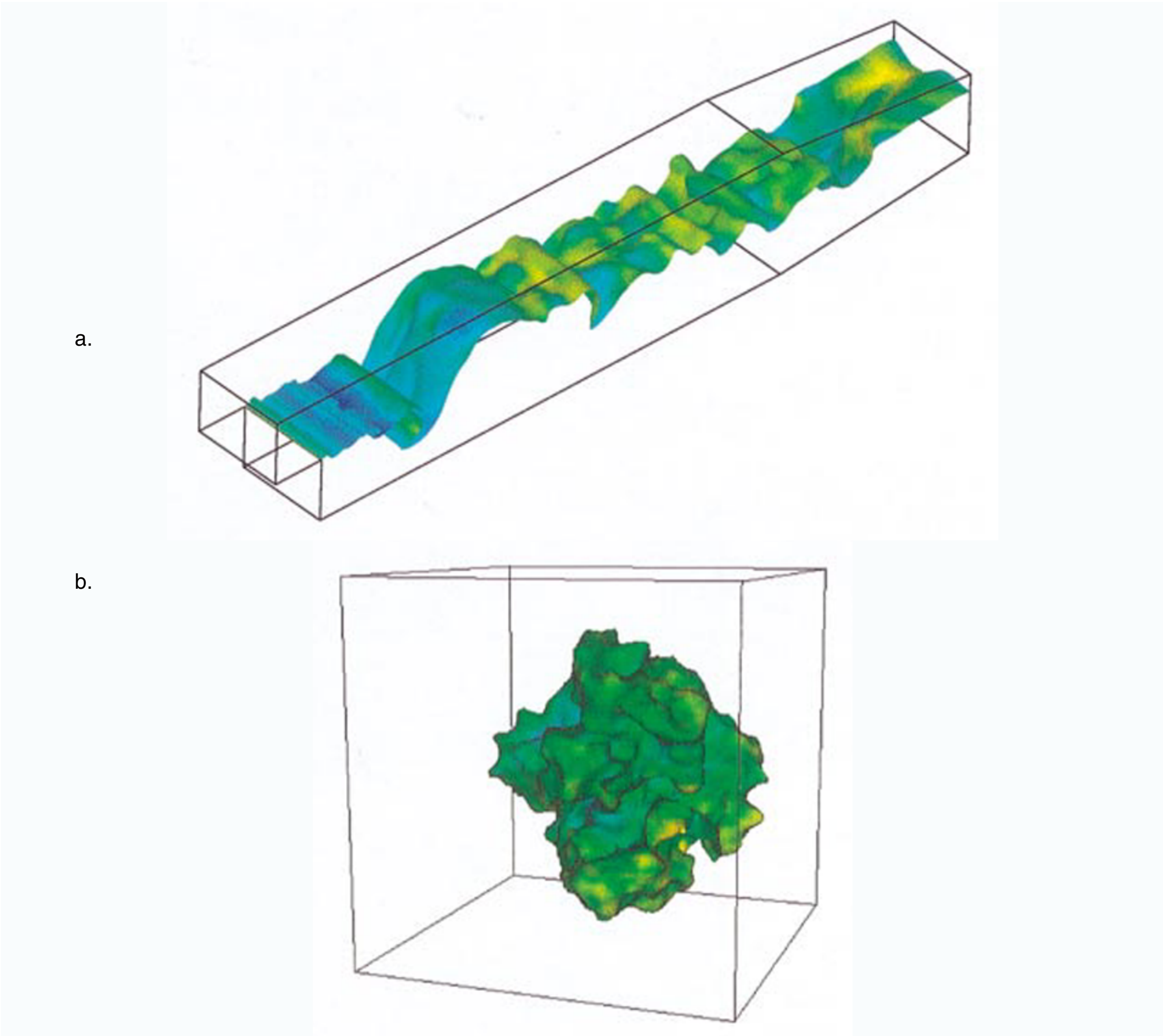

Fig. 4.

320 000 cells with the mesh appropriately refined in the shear layer. No-slip boundary conditions are applied at the walls with transmissive boundary conditions at the outlet. Random fluctuations of small amplitude are used to trigger the instability of the inlet flow. Results were insensitive to the level of applied forcing.

Figure 3a-c show visualisations of the temperature, vorticity magnitude and the effective reaction rate for the backward-facing step case. The incoming cold premixed reactants mix with hot combustion products in an initial shear layer behind the step. The large strain-rates in this region delay ignition of the flame, allowing the development of Kelvin-Helmholtz instabilities which determine the initial topological structure of the vorticity. In this region just after the step occasional helical pairing of structures occurs but this can not take place further downstream where volumetric expansion and density gradient effects resulting from combustion destroy the organised growth by vortex coalescense seen in the isothermal shear layer. Heat release mainly occurs in the convecting structures which entrain cold reactants and hot products. The resulting volumetric expansion within the structures contributes to the growth of the shear layer. The longitudinal vortices develop in the "braided" region between adjacent spanwise structures. Far downstream, vortex stretching effects break down the spanwise structures, whilst the longitudinal structures maintain their coherence.

Isosurfaces of instantaneous vorticity magnitude are plotted in Fig. 3b. The isosurfaces illustrate that most of the vorticity is not contained in the large scale spanwise rollers but is in the smaller scale, faster spinning three dimensional structures. The reaction itself is mainly confined to sheet-like structures which are folded into the cores of the spanwise vortices where rapid burning takes place. This can be seen in figure Fig. 3c. Contour lines delineate the extent of the reacting surface. The longitudinal vortices appear to wrinkle the reaction sheet causing the surface to develop regions of high curvature. In the modelling the mean flame front propagation is a function of the wrinkling parameter Ξ. The isosurface of $\overline{b}$ coloured by the strained laminar flame speed, S_u (Fig. 4a.) shows the depression in this quantity just after the step (in dark blue) due to the high tensional strain rates that occur in this region. Further downstream, spanwise variations of the laminar flame speed occur as a result of the significant three dimensionality of the flow, which is also seen in the resolved wrinkling. Fig. 4b. illustrates a fully developed turbulent flame kernel with a large degree of wrinkling at both the resolved and sub-grid scales.

5. Web-based Visualisation

All the images in this paper are instantaneous 'snapshots' of the data, selected by us to illustrate points that we wish to bring out about the data. This has two deficiencies. One is the difficulty of representing the temporal component of the data. Although it is possible to show time sequences of images, a preferable approach is to generate animations of the data. Animation is best applied to continuum data such as isosurfaces, and with the low price of data storage it is easy to generate high quality results for presentations, either to play back on a computer or to store on videotape. The constraints of a printed journal rules both of these out. However the World Wide Web (WWW) provides a solution. As a group we have set up a website (http://monet.me.ic.ac.uk) to publicise and distribute our work. On this website there is a page of animations (http:// monet.me.ic.ac.uk/ projects/ combust/ JVis/ combustAnimations.html) to go with this article. The first 4 items are various animations in jpeg and mpeg format showing the kernel growth from section 3. They include an animation of the kernel growth itself, as well as pseudo-Mie and pseudo-Schlieren movies. The next 4 are of the backward-facing step, including animations of the vorticity isosurfaces and of the flame surface $\overline{b}$ coloured by various interesting quantities.

The other deficiency of a print journal for visualisation is its lack of interactivity. The images selected by the author may not correspond to what the reader wishes to see, if only because the two may have different motivations for writing and reading the paper respectively. Giving the reader the ability to interact directly with the visualisation would enhance understanding considerably. Again, the WWW provides this ability. The final visualisation on the web page is a VRML image of the flame kernel. VRML is a standard language for describing 3-d structures which permits a degree of interactivity: in this case the reader can enlarge the image and rotate it to look in detail at whichever parts of the structure are of interest. For such a simple case, this may not be too impressive, but for more complex cases it might be invaluable.

There are clearly a number of problems with web-based visualisation. One is the shear volume of data to be transferred, particularly for VRML images which are 3-d. Standardisation of software is another issue: jpeg, mpeg and VRML have been used here as they are formats which we have ready access to, but this is not necessarily true for the reader. Long-term stability and permanence of the data is also an issue. We aim to maintain our website for the foreseeable future, but this is not a cast-iron guarantee. The development of web-based journal publication also affects this issue. Many print journals are moving to include (and so archive) such enhancements to papers published in paper form. For a wholly web-based journal the distinction between the journal paper and the web enhancement evaporates, and the animations are there as long as the journal site is in existance or chooses to archive that paper. Web-based publication affects the whole publication process in many ways [Butler:1999]; distribution and publication costs become negligable for the publisher, leaving the important roles of a guarantee of quality (via stringent peer-review) and the scientific cachet of publication in a prestigeous journal as the value added by the publishing organisation.

The other distinction that will disappear is that between a producer of the data (the author, or more generally the scientist or engineer in direct control of the CFD code) and the consumer (the reader). VRML permits the user to interact directly with the images: the development of appropriate Java applets and applications could provide direct involvement with the calculation itself. Particularly if CFD codes can become more physically intuitive to use, web-based techniques could be used to control the whole calculation, subsuming the calculation into the visualisation process in a seamless manner. This would, however, require significant advances in the ease of use of CFD codes, and it is likely that some understanding of the numerical techniques involved, and their limitations, will always be necessary.

6. Conclusions

The physics involved in premixed turbulent combustion is immensely complicated, and CFD simulation of even the simplest cases involves detailed modelling and high computational effort. Nevertheless such simulation is worthwhile, because of the extreme importance of such flows industrially. Visualisation of the results of the simulations has three main roles to play. Firstly, it can help to understand the behaviour of the models, in terms of the interaction between the various parameters. This has been explored in section 4. Secondly, by generating images to resemble the results of experimental imaging techniques, such as Mie or Schlieren photography, we can validate the models more easily, at least at a qualitative level. Finally, the visualisation can be used as a tool to understand the physics at a deeper level. Simulations can go further than experiments in this manner, as it is possible to generate data for quantities of interest directly (such as reaction rates or length scales), which are either difficult to measure or have to be deduced from experimental techniques such as Schlieren. Thus such simulations, and their visualisation, can be a valuable tool for research and engineering in the field of turbulent combustion.

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David Gosmam: He graduated from the University of British Columbia in 1962 with the degree of Bachelor of Applied Science in Chemical Engineering. He then joined the Mechanical Engineering Department, Imperial College where he performed PhD studies in two-phase flow. Following this he became a member of academic staff and now holds the position of Professor of Computational Fluid Dynamics. He is also a director of a company which produces industrial thermofluids analysis software. He has been active in the field of computational fluid dynamics for more than twenty years, is co-author of several books and around 150 technical papers on the subject, and acts as a consultant in this area to numerous organisations. His main research interests are in the development and application of general prediction methods for steady and unsteady single- or multi-phase flows, with possible accompanying heat and mass transfer.