**Computational simulation and modelling of turbulent reacting flows**

**General Scope of the work**

Turbulent combustion is a subject of great importance and relevance in the present scenario of engineering science. Conversion of chemical energy to sensible energy (heat) by means of a combustion process in a turbulent flow environment is related to many urgent energy efficiency and pollutant emission issues of worldwide concern. Thus a fundamental understanding of the basic phenomena of combustion is essential for improving the efficiency, reliability, safety and environmental pollution control aspects of combustion systems. In many practical combustion applications, the combustion takes place in a turbulent environment in such a manner that the reactants are fully premixed before being burnt in the device (e.g. industrial Gas Turbines and Spark Ignition (SI) engines). This gives better control over the chemistry of the combustion process, which in turn has major implications from the point of view of reducing pollutant emission. Recent pollution control regulations have further increased the importance of premixed combustion. Premixed combustion is presently very much in use in stationary gas turbines; it is further anticipated that it will be the principal energy-releasing mechanism in aero-engines within next ten years (private communication Rolls Royce plc.).

The extent to which combustion performance can be improved while simultaneously reducing fuel consumption and pollutant emissions are limited by available design and analysis tools. Computational Fluid Dynamics (CFD) based tools have become indispensable in this respect because a considerable amount of time and expensive experimentation can be saved with the help of an efficient CFD analysis.

Fundamental understanding of complex problems such as turbulent combustion events is aided significantly by computational modelling and simulation. A model presents a simplified way of predicting and describing physical phenomena. For simulations of a typical combustion device to be feasible, even on the largest of computers, the inclusion of simplifying models is required. However most of the CFD tools used in industry for analysing turbulent reacting flows rely on the Reynolds Averaged Navier Stokes (RANS) technique where the averaged (mean) behaviour of the flow field is obtained as the solution. In this method the instantaneous behaviour of flow character and flow features associated with different length scales are smeared out because of the averaging process, which can be seen from an example presented in Figure 1. Often strong *ad hoc* assumptions are invoked in order to model the lost information.

Recovering some of the lost information necessitates a new genre of flow modelling called Large Eddy Simulation (LES) where some of the instantaneous flow features can be retrieved as a part of the solution. In LES, large-scale flow structures can be obtained from the simulation without any modelling approximation, but small-scale physics taking place at the sub-grid level is modelled. In recent years, improved computational capacity has made it possible to carry out Direct Numerical Simulations (DNS) of a turbulent flame without any kind of physical approximation. DNS datasets can be treated as an equivalent of controlled experimental data, which has significantly increased the understanding of turbulent combustion during the last decade. As DNS is far too expensive for industrial use, LES is used instead; however DNS data is important for efficient RANS and LES modelling.
Figure 1: Principles of DNS, LES and RANS. (a) Instantaneous view of a flame surface ($c = 0.8$), (b) LES filtered flame surface for a filter size equal to two times of laminar flame thickness ($\tilde{c} = 0.8$), (c) Reynolds averaged flame surface ($\langle c \rangle = 0.8$). Figures are based on the DNS simulations by Chakraborty and Cant (2003-2004).

**Direct Numerical Simulation (DNS) of turbulent premixed flames**

In this research programme, three-dimensional DNS simulations of turbulent premixed flames are carried out in statistically planar and spherical configurations under decaying turbulence. Until recently limitation of computational capacity allows for DNS either in two-dimensions with detailed chemistry, or in three-dimensions with simplified chemistry. For my research the second approach is often favoured, as turbulent flow is intrinsically three dimensional in nature. The simulation parameters for DNS simulations are judiciously chosen in order to carry out a systematic numerical experiment to examine the effects of turbulence intensity, heat release and the relative strength of heat and species diffusion (differential diffusion due to non-unity Lewis number) on premixed flame propagation. The DNS data is subsequently used for turbulent reaction rate modelling in the context of Reynolds Averaged Navier Stokes (RANS) and Large Eddy Simulations (LES).

Reaction rate modelling is the most challenging task in turbulent combustion studies. Due to the highly non-linear nature of the reaction rate expression, conventional averaging/filtering technique cannot be used to model the mean chemical reaction rate. Flame Surface Density (FSD) based modelling is one of the most popular and established techniques for reaction rate closure in turbulent premixed flames within the context of RANS, where the reaction rate modelling is translated into the modelling of turbulent flame surface area to volume ratio (which is known as FSD in combustion literature). FSD based modelling in the context of LES is relatively recent.

In this research programme DNS data is analysed in order to understand the statistical behaviour of flame propagation speed in response to local strain rate and curvature. This information is subsequently used to carry out an *a-priori* DNS analysis of FSD based combustion models in the context of RANS and LES. The performance of existing models is analysed in comparison to DNS data. Based on this assessment, modifications to the existing models are suggested and new models are proposed wherever necessary. Finally all the information is drawn together to propose a modelled FSD transport equation, which is capable of addressing the flame propagation behaviour properly in both the corrugated flamelets and the thin reaction zones regimes. However, an extra transport equation immensely increases the cost of RANS/LES simulation and there is little motivation behind using the FSD transport equation model except in specialised applications (i.e. combustion instabilities in gas turbines). In this research the knowledge acquired in previous studies to construct an algebraic expression based FSD model, which will be less computationally intensive in nature. For this purpose DNS data of turbulent premixed flames are used for assessing the performance of existing algebraic FSD models based on *a-priori* DNS analysis. It is anticipated that the present study will lead to modification of the existing algebraic FSD models and development of a new model if necessary. DNS
data was explicitly Reynolds averaged/LES filtered using Gaussian filter. Finally the performance of
the newly developed model has been assessed alongside other models in comparison to the filtered
DNS data. The model developed based on this study will be valid both in the corrugated flamelets
regime as well as in the thin reaction zones regime. The performance of the newly developed models
has been demonstrated to be comparable if not better than the existing algebraic models of FSD.

The FSD is also closely related to the scalar dissipation rate in turbulent premixed flames. Modelling of
turbulent flame propagation using the scalar dissipation rate is well established in the context of non-
premixed flames. Relatively little has been done on scalar dissipation rate based combustion modelling
for turbulent premixed flames. However, the scalar dissipation rate is closely related to the mean
chemical reaction rate in turbulent premixed flames. In this research, the FSD modelling information is
used to propose a model for scalar dissipation rate transport in turbulent premixed flames in context of
RANS to start with. The extension of this scalar dissipation rate model to LES is also indicated for the
first time in the context of turbulent premixed flames. A unified scalar dissipation rate transport
equation based reaction rate closure is proposed based on this research, which is valid both in the
corrugated flamelets and the thin reaction zones regimes. The possibility of extending this scalar
dissipation rate modelling in the context of LES is also indicated for the first time. It is planned that the
scalar dissipation rate modelling will be extended for LES based on the fundamental understanding
gained from this research programme.

This research for the very first time demonstrated that turbulent scalar gradient may align preferentially
align with the most extensive principal strain rate in contrast to the preferential alignment of passive
scalar gradient with the most compressive principal strain rate. Detailed physical explanations for the
above behaviour has been provided in detail and this physical information have been used to propose
the strain rate related terms in the FSD and scalar dissipation rate transport equation.

It has been also shown for the very first time that Lewis number has a significant influence on turbulent
flux behaviours in turbulent premixed flames. Turbulent fluxes of scalar, scalar gradient, scalar
variance and turbulent kinetic energy have been demonstrated to show counter-gradient transport for
flames with Lewis much smaller than unity whereas gradient transport has been observed for the
similar turbulence conditions in the unburned gas for the flames with Lewis number close to unity. A
unified modelling strategy has been developed in the context of RANS, which can be used for turbulent
reaction closure of turbulent premixed flames with non-unity Lewis numbers for the very first time.

Relevance of this work

The models developed during the course of this research programme are expected to perform better
than the existing FSD and scalar dissipation rate based models, especially under unsteady combustion
situations where the dynamic effects of strain rate and curvature on flame propagation are significant.
This situation is very common in combustion instabilities. Thus, this work in turn can help in designing
efficient combustion systems in practical engineering applications; for example in gas turbine
combustors, LES can be useful in analysing the large-scale flow features responsible for combustion
instabilities which may give rise to self-sustained oscillation and lead to structural failure.

Principal Investigator

Prof. Nilanjan Chakraborty in collaboration with (i) Cambridge University Engineering Department;
(ii) Imperial College London; (iii) Sandia National Laboratory, USA; (iv) University of Darmstadt,
Germany; (v) University of New South Wales, Australia; (vi) Chalmers University, Sweden

Research Funding

Engineering and Physical Sciences Research Council (EPSRC), UK
DNS simulations of (a) statistically planar back-to-back, (b) statistically spherical turbulent premixed flames.

DNS of stratified charge combustion

In a number of engineering combustion devices, at the time of ignition the fuel and oxidiser are neither fully separated (i.e. non-premixed combustion) nor homogeneously mixed (i.e. premixed combustion) and this situation is commonly referred to as stratified mixture combustion. Stratified mixture combustion has applications ranging from Gasoline Direct Injection (GDI) engines to Lean Premixed Prevaporised (LPP) gas turbines as well as Homogeneous Charge Compression Ignition (HCCI) engines where the first qualifier is rarely met in practice. Recent studies of stratified mixture combustion have found that the global heat release can increase as a result of mixture stratification under some conditions in comparison to the corresponding perfectly premixed case, whilst decreasing under other conditions. Stratified mixture combustion has the potential to offer sustained globally fuel-lean combustion, hence reducing fuel consumption particularly at light-load, low-speed operations in automobile applications. Furthermore, in globally fuel-lean combustion the likelihood of high temperature locations decreases considerably, which leads to a significant reduction in NOx emissions. Moreover, an increase in fuel efficiency of up to 25% and 30% has been observed in GDI and HCCI engines respectively. Therefore an accurate and efficient method of predicting the behaviour of stratified mixture combustion is desirable and, in turn, will contribute to the development of higher efficiency, lower emission combustion devices.

In this research programme, three-dimensional Direct Numerical Simulations (DNS) with simplified chemistry, appropriate for the combustion of realistic hydrocarbon fuels, have been carried out for a variety of mixing fields and turbulence intensities to enhance the present state of fundamental understanding and to create a database for the assessment of existing combustion models and to develop new models wherever necessary. Three-dimensional DNS of turbulent combustion of stratified mixtures, with a reasonably complex chemical mechanism dictated by computational economy, have been carried out to validate the qualitative findings obtained from simplified chemistry based DNS data. The second part of the project involved the development of a combustion model mainly in the context of Reynolds Averaged Navier Stokes (RANS) simulations, but the possible extensions of RANS models for Large Eddy Simulations (LES) are also suggested. The newly developed models have been implemented into an industry-standard Computational Fluid Dynamics (CFD) package so that they can then be used for future engineering design purposes. The specific objectives of this research programme are as follows:

1. To examine stratified charge combustion through three-dimensional Direct Numerical Simulations (DNS). These results provide:
   (i) Fundamental insight into the physical processes occurring during the combustion of mixtures with strong thermal and species inhomogeneities.
   (ii) A DNS database that has been used for model validation and new model development. Moreover, the developed DNS database will continue to work as an important source for the community for model development and this DNS database will be shared with interested UK and international researchers.

2. To develop and validate models for turbulent stratified charge combustion, which will provide the following:
(i) Assessment of existing turbulent combustion model performances for partially premixed combustion based on a-priori analysis of DNS data.

(ii) Identifying the strengths and limitations of the simplified chemistry based models for HCCI combustion (e.g. Multi-zone model) which are in use in automobile engine design in the light of DNS data analysis.

(iii) Development of new models/sub-models for turbulent stratified charge combustion in the context of Reynolds Averaged Navier Stokes (RANS) and suggestion of their extensions to Large Eddy Simulations (LES), which can also be used for accurate predictions of flame propagation behaviour, combustion performance and pollutant emission characteristics.

During the course of this research programme three-dimensional DNS databases of freely statistically planar turbulent flames propagating through stratified mixtures have been generated for different configurations for different values of global mean equivalence ratio, root-mean-square equivalence ratio, global Lewis number and turbulent velocity fluctuations, integral length scales of turbulent velocity fluctuations and equivalence ratio fluctuations. This provides a wealth of important information, which can be used for the purpose of assessing existing models and develop new models in the context of RANS and LES. The database developed during the course of this project will continue to be a very useful source of information for gaining fundamental understanding and model development in the future. This DNS database is subsequently used to assess the performance of the existing algebraic models for scalar variances, co-variances, dissipation rates and cross-dissipation rates. The existing models that are the best suited for predicting the relevant quantities are identified and for some quantities either new algebraic models were proposed or existing models were modified, when existing models were found to predict the quantities in question adequately. Transport equation based closure for some quantities where algebraic models are found not to perform well. Models have been proposed for all the terms for the transport equations of fuel mass fraction variance, co-variance of fuel mass fraction and mixture fraction fluctuations, scalar dissipation rates of mixture fraction and fuel mass fraction and the cross scalar dissipation rates of fuel mass fraction and mixture fraction fluctuations in the context of RANS. The quantities such as variance, co-variance, scalar dissipation rate and cross-scalar dissipation rate play pivotal roles in the reaction rate closure in turbulent combustion of stratified mixtures. The aforementioned modelling activity aided by DNS data devised a coherent unified modelling methodology which can be used for reaction rate closure both high and low Damkohler number conditions. This modelling exercise was also closely related to the modelling turbulent premixed combustion because it is a special case of turbulent stratified combustion modelling. As a result of this, significant advances in different aspects of scalar dissipation rate, Flame Surface Density (FSD) and scalar flux modelling of turbulent premixed flames. The statistics of flame propagation statistics in turbulent inhomogeneous mixtures have been studied in terms of displacement speed and its components and FSD based reaction rate closure has been extended for turbulent combustion of stratified mixtures for both high and low Damkohler number conditions in the context of RANS. The possible extension of the RANS models for the purpose of LES is also identified.

The DNS data also has been used to identify the strengths and limitations of the simplified models for combustion (e.g. Multi-zone model) which are in use in analysing DNS data of localised ignition of thermally inhomogeneous mixtures, which is often realized in Homogeneous Charge Compression Ignition (HCCI) engines.

In addition, the models and findings have been shared with the Combustion Research Group in Cambridge (especially with Profs. R. Stewart Cant, E. Mastorakos and Dr. N. Swaminathan) who are also engaged in computational and experimental analysis of turbulent combustion of stratified mixtures.

Relevance of this work

This work for the first time provides a modelling methodology for the turbulent stratified charge combustion, which is validated using a-priori DNS analysis. Moreover, the developed models are proposed in such a manner that these models can be applied in the limits of fast and slow chemistry in contrast to the existing methodology which is only valid in the fast chemistry limit. However, in IC engines and gas turbine applications slow chemistry limit can be encountered especially when fuel-lean combustion is involved. Thus the above research activity is important for the purpose of development of a coherent Computational Fluid Dynamics (CFD) modelling methodology which can help in designing new generation GDI, HCCI engines and gas turbine combustors which operate using stratified mixtures.
**Principal Investigator**

Prof. Nilanjan Chakraborty in collaboration with (i) Cambridge University Engineering Department; (ii) Imperial College London; (iii) Sandia National Laboratory, USA; (iv) University of Liverpool

**Research Funding**

Engineering and Physical Sciences Research Council (EPSRC), UK

(a) Field of fuel mass fraction of a statistically planar turbulent stratified flame at the central mid-plane. The white lines show reaction progress variable contours from 0.1 to 0.9 from left to right in steps of 0.1. (b) The reaction progress variable isosurface for this flame where chemical reaction progressed to 80% completion. The isosurface is coloured by local equivalence ratio.

**DNS of spark ignition of inhomogeneous mixtures**

Spark Ignition (SI) in homogeneous reactants has been studied extensively in the context of SI engine combustion. However, spark ignition in inhomogeneous reactants has applications in gas turbine relight applications. In order to increase the effectively of the spark ignition in aero-engines, the underlying physics of the flame propagation following spark ignition event in inhomogeneous reactants needs to be understood. This understanding in turn can help in modelling the spark ignition event, which can eventually be applied for the analysis of relevant engineering systems. In comparison to the vast body of literature on spark ignition in premixed charge relatively little has been done both experimentally and numerically on spark ignition in inhomogeneous mixtures. Ignition probability in spark ignition in inhomogeneous reactants has been experimentally studied in the past. However, those studies were motivated by the safety concern so the flame propagation behaviour following ignition was beyond the scope of this study. Experimental studies characterised spark parameters such as spark energy, critical radius of hot gas kernel, and spark duration for successful spark ignition in inhomogeneous reactants. However, in order to model a practical spark ignition application in inhomogeneous mixtures such as high altitude relight in gas turbine applications one needs sufficiently accurate experimental and Direct Numerical Simulation data based on which the Computational Fluid Dynamics (CFD) models can be devised and the model parameters can be calibrated. In recent days Direct Numerical Simulation (DNS) has become an important tool for physical understanding of turbulent combustion phenomena. In DNS a small element of the flow domain is simulated where the smallest relevant length and time scales of turbulent combustion process are adequately resolved as a result of which no physical model is required to address the concerned turbulent combustion process. DNS data can effectively be treated as an experimental data with infinite resolution. Moreover, effects of a number of different parameters can be studied independent of each other with relative ease by doing carefully devised numerical experiments with the help of DNS.
In order achieve the above objective three-dimensional compressible DNS simulations have been carried out for spark ignition in inhomogeneous mixtures under turbulent environment using a DNS code. This study focuses only on the thermal aspects of the spark ignition. The electrical aspects of spark ignition are beyond the scope of this study. With the present day computational power, it is almost impossible to take into account both the aspects of three-dimensionality of turbulence and detailed chemistry in DNS simulations. As turbulent flow is inherently three-dimensional in nature the simulations are carried out in three dimensions with one-step irreversible Arrhenius type chemistry. The thermal effects of spark ignition are accounted for by an extra source term in the energy source term, which essentially deposits a given amount of spark energy over a prescribed spark duration time. Spark location is varied across a statistically one-dimensional mixing layer so that the spark centre can be changed from stoichiometric mixture to either fuel-rich or fuel-lean mixtures. Special care has been taken to resolve both the mixture fraction and thermal gradients in addition to the smallest length scale of turbulence. A number of simulations have been carried out for different spark powers, turbulent velocity fluctuation levels, initial mixing layer profiles and spark locations.

This study is the first comprehensive study where the flame structure and propagation following successful ignition of inhomogeneous reactants is comprehensively studied. It has been found that In the case of successful ignition, the flame shows a tribrachial (triple flame) structure. At later stages of flame propagation, the lean premixed branch and the diffusion flame stabilised along the stoichiometric mixture fraction isosurface may come close to each other and may eventually merge. The above analysis clearly indicated the successful performance of spark ignition is dependent on (i) level of turbulence, (ii) fuel gas fraction gradient and (iii) the local equivalence ratio of the fuel-air mixture. An optimum combination of the above three parameters ensures a successful spark ignition. This clearly indicates the design requirements of spark ignition system and its location in gas turbine combustor in order to achieve an efficient high altitude relight performance in aero-engines. Moreover, this DNS data has been analysed for understanding turbulent scalar flux transport in the context of Conditional Moment Closure (CMC) model. This is believed to be the first study where scalar transport modelling has been attempted in the context of CMC and a new transport equation is derived for conditional turbulent scalar flux.

Further, the edge flame propagation statistics of the edge flame arising out from localised ignition of inhomogeneous reactants have been studied extensively based on DNS data. The non-linear dependence of edge flame displacement speed on local scalar dissipation rate and curvature has been explained for the first time.

Recently this study has been extended to understand the effects of mixture fraction value and the magnitude of its gradient at the ignitor location on the localised ignition of turbulent mixing layer. It is shown that the reaction rate of fuel is found to be greater in the fuel rich side and localised ignition by placing the ignitor at a fuel-lean region may initiate ignition but it may eventually lead to extinction as the diffusion of heat from the hot gas kernel may overcome the heat release due to combustion. It is demonstrated that ignition in the fuel lean region may fail for an energy input for which self-sustained flame has be en achieved in the cases of igniting at stoichiometric and fuel-rich locations. It is found that the fuel reaction rate magnitude is negatively correlated with density-weighted scalar dissipation rate in the most reactive region. An increase in the initial mixture fraction gradient at the ignition centre for the ignitor placed at stoichiometric mixture decreases the spreading of the burned region along the stoichiometric mixture fraction isosurface. By contrast, the mass of the burned region increases with an increase in the initial mixture fraction gradient at the ignition location, as for a given ignition kernel size the thinner mixing layer includes more fuel-rich mixture, which eventually increases the overall burning rate than that compared to a thicker mixing layer where relatively smaller amount of fuel-rich mixture is engulfed within the hot gas kernel.

Until recently most combustion DNS studies were carried out in canonical configurations under decaying turbulence. Recent advances in computational hardware have made it possible to carry out DNS of relatively complex flows with engineering relevance. Turbulent jet flows are extremely relevant to engineering applications and at the same time can be simulated with the help of DNS. In Nuffield Foundation funded project an igniting turbulent planar co-flowing jet has been simulated using three-dimensional DNS. The jet issuing from a rectangular slot is fuel-rich whereas the co-flow is fuel-lean. The chemical mechanism is described by a single step irreversible reaction. The strain rate effects on the density weighted displacement speed of the edge flame resulting from localised ignition have been studied in detail in terms of the strain rate responses of its reaction, normal diffusion and
tangential diffusion components. It is demonstrated that the strain rate effects on the magnitude of fuel mass fraction gradient affect the reaction and normal diffusion components of density weighted displacement speed. The strain rate response of density weighted displacement speed is found to be consistent with previous experimental studies. The effects of differential diffusion due to non-unity Lewis number of the fuel on the overall localised ignition performance and on the edge flame propagation characteristics in turbulent environments are analysed in detail for the first time in this research programme.

It is also planned that this study will be extended for droplet-laden flows where both liquid and gaseous phase will simultaneously be present and the level of gaseous mixture inhomogeneity will be altered locally by the rate of evaporation. Moreover, it is planned that DNS in three-dimensions will be carried out in near future in the presence of realistic chemistry for hydrocarbon fuels, which is presently rare in combustion literature.

Relevance of this work:

Spark ignition in inhomogeneous reactants has its use in gas turbine relight applications and Direct Injection (DI) system in automobile industry. The DI engines are becoming increasingly important in the context of present pollution control regulations because of its low pollutant emission level in comparison to conventional engines. It is expected that the physical insight grained from the present study will be immensely useful in designing spark ignitor system in new generation DI engines.

Principal Investigator

Prof. Nilanjan Chakraborty in collaboration with (i) Cambridge University Engineering Department; (ii) University of Darmstadt; (iii) University of Liverpool

Research Funding

Engineering and Physical Sciences Research Council (EPSRC), UK

Fields of (a) fuel mass fraction, (b) normalised temperature and (c) fuel reaction rate magnitude at the central mid-plane just after localised ignition of turbulent mixing layers obtained based on three-dimensional DNS simulations. The white line in Fig. 2c shows the stoichiometric mixture fraction contour.
Fig. 4: Fields of (a) fuel mass fraction and (b) non-dimensional temperature at the central mid-plane just after localised ignition of turbulent planar stratified jet based on three-dimensional DNS simulations. The broken line shows the stoichiometric mixture contour.