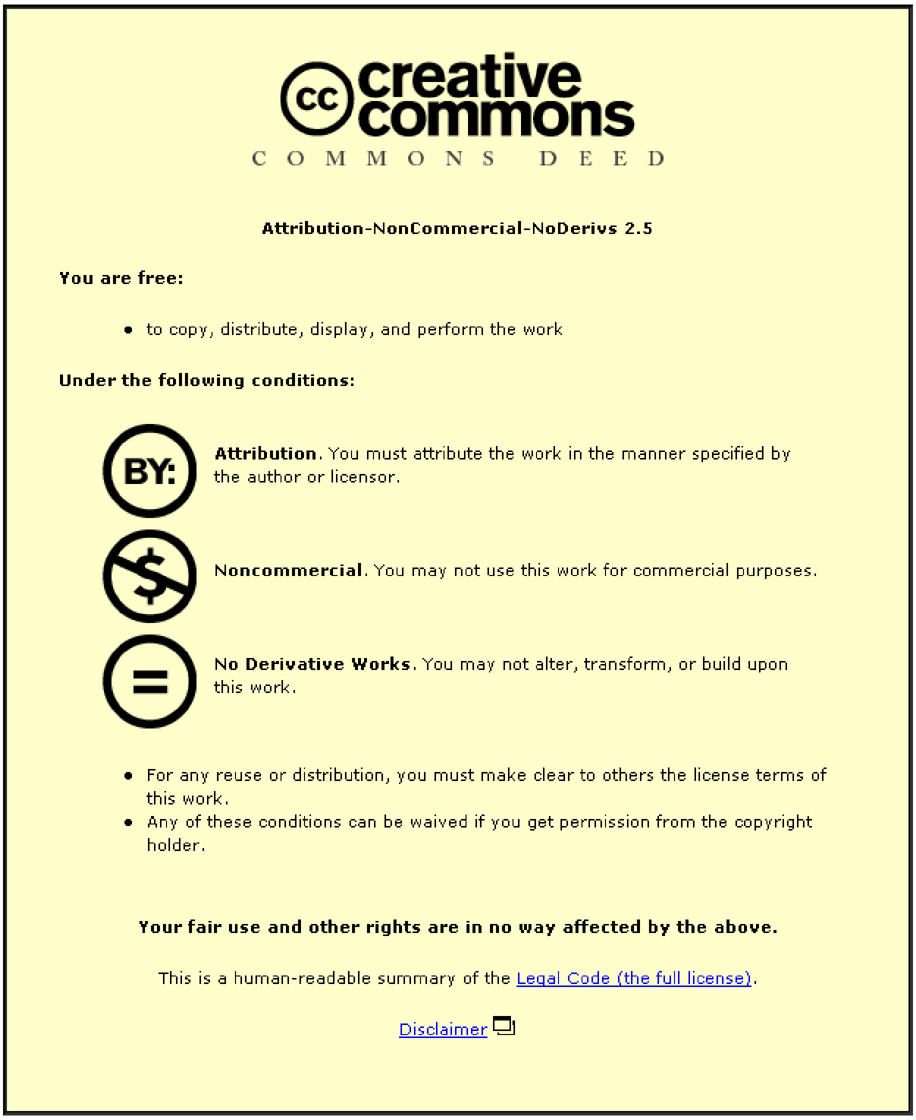

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Evaluation of Turbulence/Radiation Effects using LES Combustion Simulation Data

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Abstract

This paper describes the evaluation of turbulence/radiation effects on a swirl flame. The data obtained from a LES calculation in this case provides time-varying temperature field and species concentrations contributing to radiation fluctuations. In the radiation calculations demonstrated here, time varying data obtained from the LES calculations are post processed using the Discrete Transfer method incorporating a radiative property calculation algorithm to obtain radiation fluctuation statistics. The study provides an insight into how radiation fluxes, absorption coefficients and radiation intensities fluctuate in a highly turbulent complex practical flame. Simulation results show that temperature self correlation can be as high as 4 times and turbulence fluctuations has a very significant effect on source term calculations.

1. Introduction

Advancement in the design and operation of combustion devices used in automobile, air transport and power generation industries is very important for the reduction of emissions contributing to global warming. The drive is to make combustion equipment to operate at higher efficiencies so that more power could be extracted for the same amount of fuel burnt in the past. This would, in the long run, reduce emissions or maintain at the present level while meeting the present and future demand for power/energy. To this end Computational Fluid Dynamics (CFD) has a major role to play and more and more industries are now using CFD to explore flow behaviour of various designs and simulate temperature, heat transfer and emissions in combustion equipment before prototypes are built for testing. Such CFD studies have various benefits – design cycle can be shortened, new ideas can be tested without prior experimentation which can be very costly and incremental changes can be made to the design to achieve a desired effect.

CFD models for combustion simulations are, however, far from perfect to use in such studies. There are many issues which makes combustion modelling one of the most difficult areas in CFD applications. Complexities such as turbulence/chemistry interactions, chemical kinetics, coupling of flow turbulence and temperature to density, heat transfer and radiation effects makes CFD modelling of combustion very difficult. Radiation is often neglected in numerical simulations of many combusting flows. The reason being the computational effort needed to model radiation and the complexities (coupling) involved. Inclusion of radiation effects in combustion models is very important to achieve good accuracy in combustion modelling and for the estimation of correct wall heat transfer in the equipment design. In many practical situations fluctuations of radiation arising from the fluctuation of temperature and absorption coefficients can be very important where combustion characteristics and chemistry effects contribute to combustion instabilities, extinction and re-ignition effects. In this paper LES based combustion modelling for non-premixed combustion is considered for detailed evaluation of fluctuating radiation effects. In the radiation calculations considered here, time varying data obtained from LES are post processed using the Discrete Transfer (DT) method incorporating an absorption property calculation algorithm to obtain radiation fluctuation statistics. The study provides an insight into how radiation fluxes, absorption coefficients and radiation intensities fluctuate in a highly turbulent complex practical flame.

Fluctuations of radiation have been recognised in a number of studies [1-15]. In a theoretical approach Cox [8] showed that in flames, channelled under a corridor ceiling, the radiant intensity can easily be increased by 24% due to turbulent fluctuations. Experimental and numerical work of Faeth et al [9], Gore and Faeth [10], Kounalakis et al [11] have shown that fluctuation of radiation quantities can be as much as 100% of the mean values. The work of Nelson [12] showed that TRI effects are dominated by temperature fluctuations. The work of Kiritzstein and Soufiani [13] also shows that radiative intensities increase with increasing turbulent fluctuations while the effect of concentration fluctuations had weak effect on radiative intensities. A comprehensive review of many turbulence radiation interaction researches has been published by Coelho [14] and the paper summarises many other studies which have attempted to study TRI. Among these there are many modelling attempts. Modelling and numerical quantification of TRI is difficult in the absence of transient data. Mazumder and Modest [15] for example used pdf equations and the Monte Carlo method in a methane-air diffusion flame and showed that inclusion of absorption coefficient-temperature correlation increase radiative heat flux by 40-45%. Further studies of Modest and co-workers [16-18] using DNS coupled with Monte Carlo method in idealised non-premixed flame situation show that contributions from temperature self correlation, absorption coefficient-Plank function correlation and absorption coefficient-intensity correlation are important and the relative contribution varies with optical thickness. Using simulated flame conditions Coelho [14] has shown that turbulent fluctuations contribute to decrease in flame temperature below the level observed without radiation fluctuations and the net power and the fraction of radiative heat loss increase due to TRI.

The work reported in this paper attempts to quantify TRI effects using LES data in a real flame. The flame considered is from the Sydney University swirl burner experimental program on non-premixed flames. This paper first describes the validation of LES combustion models for a selected flame where swirl stabilised combustion is modelled and compared with high quality experimental data to demonstrate capabilities of the LES methodology. In the validation of LES, experimental data is used to compare important variables such as flow velocities, their rms fluctuations, mixture fraction, and its fluctuations and species concentrations for major and minor species. The data obtained from the LES calculation in this case provides time-varying temperature field and species concentrations contributing to radiation fluctuations. It should be noted that the radiation data and statistics presented here are not a coupled calculation but gives very important parameters to identify TRI effects. The study conducted here is very much an exploratory study to understand radiation fluctuation effects and further work to incorporate radiation into a fully coupled LES calculation is underway.

In the following sections we describe some details of the LES and radiation calculation method used to simulate the chosen swirl flame. Further details of the experimental configuration and boundary conditions used in our simulations are then described. We present some comparisons of the LES predictions with the experimental data to show that LES prediction used in the radiation study are in good agreement with data. The mean and instantaneous data from the LES calculations are used as an input for the radiation calculation. Using the transient LES data, the DT method and a coupled radiative property algorithm we calculate the transient behaviour of radiation and present radiation results for this swirling flame and discuss TRI effects.

2. Mathematical Model

2.1 Equations solved

Large eddy simulation demonstrates accurate and more sophisticated methodology for turbulence calculations compared to Reynolds Averaged Navier Stokes (RANS) based modelling. LES resolves the large scale turbulent motions which contain the majority of turbulent kinetic energy and control the dynamics of turbulence, whereas the small scales or sub-grid scales are modelled. The advantage of resolving the large scale motion is not applicable to chemical source term as the chemical time scales are smaller and therefore combustion needs to be modelled. However, LES seems to have the advantage due to its ability to predict accurately the intense scalar mixing process in any complex flow. In this work we use the Steady Laminar Flamelet Model (SLFM) with LES to form the combustion modelling aspect with turbulence. Further details of the model can be found in [19-21].

In LES the governing equations resolve the large scale features, which must be obtain by applying the filtering operator. The filtered field $\overline{f(x,t)}$ is determined by convolution with the filter function G.

$$\overline{f}(x) = \int_{\Omega} f(x')G(x-x',\overline{\Delta}(x))dx' \tag{1}$$

Where the integration is carried out over the entire flow domain Ω and $\bar{\Delta}$ is the filter width, which varies with the position. A number of filters are used in LES and a top hat filter having the filter-width $\bar{\Delta}_j$ set equal to the size Δx_j of the local cell is used in the present work. In turbulent reacting flows large density variation occurs and that is treated using Favre filtered variables. The transport equations for Favre filtered mass, momentum and mixture fraction are given by

$$\frac{\partial\bar{\rho}}{\partial t}+\frac{\partial\bar{\rho}\tilde{u}_j}{\partial x_j}=0 \tag{2}$$

$$\frac{\partial\bar{\rho}\tilde{u}_i}{\partial t}+\frac{\partial(\bar{\rho}\tilde{u}_i\tilde{u}_j)}{\partial x_j}=-\frac{\partial\bar{P}}{\partial x_i}+\frac{\partial}{\partial x_j}\left[\bar{\rho}\nu\left(\frac{\partial\tilde{u}_i}{\partial x_j}+\frac{\partial\tilde{u}_j}{\partial x_i}\right)-\frac{2}{3}\bar{\rho}\frac{\partial\tilde{u}_k}{\partial x_k}\right]+\frac{\partial\tau_{ij}}{\partial x_j} \tag{3}$$

The transport equation for conserved scalar mixture fraction is written as

$$\frac{\partial\bar{\rho}\tilde{f}}{\partial t}+\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\tilde{f}\right)=\frac{\partial}{\partial x_j}\left[\bar{\rho}\left(\frac{\nu}{\sigma}+\frac{\sigma_t}{\sigma_t}\right)\frac{\partial\tilde{f}}{\partial x_j}\right] \tag{4}$$

In the above equations ρ is the density, u_i is the velocity component in x_i direction, p is the pressure, ν is the kinematics viscosity, f is the mixture fraction, ν_t is the turbulent viscosity, σ is the laminar Schmidt number, σ_t is the turbulent Schmidt number. An over-bar describes the application of the spatial filter while the tilde denotes Favre filtered quantities. The laminar Schmidt number was set to 0.7 and the turbulent Schmidt number for mixture fraction was set to 0.4.

2.2 Turbulence Model

The subgrid contribution to the momentum flux is computed using Smagorinsky eddy viscosity model [22], which uses a model constant C_s, the filter width Δ and strain rate tensor $S_{i,j}$ according to equation (5):

$$\nu_t=C_s\Delta^2\left|S_{i,j}\right|=C_s\Delta^2\left|\frac{1}{2}\left(\frac{\partial\tilde{u}_i}{\partial x_j}+\frac{\partial\tilde{u}_j}{\partial x_i}\right)\right| \tag{5}$$

The model parameter C_s is obtained through the localised dynamic procedure of Piomelli and Liu [23].

2.3 Combustion Model

In modelling combustion, the chemical reactions occur mostly in the sub-grid scales and therefore consequent modelling is required for combustion chemistry. Here a presumed probability density function (PDF) of the mixture fraction is chosen as a means of modelling the sub-grid scale mixing. A β function is used for the mixture fraction PDF. The functional dependence of the thermo-chemical variables is closed through the steady laminar flamelet approach. In this approach the variables, density, temperature and species concentrations only depend on Favre filtered mixture fraction, mixture fraction variance and scalar dissipation rate. The sub-grid scale variance of the mixture fraction is modelled assuming the gradient transport model proposed by Branly and Jones [24]. The flamelet calculations have been performed using the Flamemaster code [25] incorporating the GRI 2.11 mechanism for detailed chemistry (Bowman et al.[26]).

2.4 Radiation Model

The governing radiative transfer equation is of integro-differential nature which makes the analysis difficult and computationally expensive. The well known Discrete Transfer Method (DTM) [27,28] is used as the radiation calculation algorithms in this work. This is a ray-based calculation method and in our previous work we have established the accuracy and advantages of this method when applied to large and complex problems [29-31].

The discrete transfer method is based on solving radiative transfer equation (RTE) for some representative rays fired from the boundaries. Rays are fired from surface elements into a finite number of solid angles that cover the radiating hemisphere about each element and the main assumption of the DTM is that the intensity through solid angle is approximated by a single ray. The number of rays and directions are chosen in advance. In the DT method RTE is solved for each ray from one solid boundary to another solid boundary in the geometry. Rays fired from solid surface boundaries and traced through the volume. The calculation of radiation source term is based on the distance travelled in each control volume. At the boundaries radiative heat transfer boundary conditions are used to determine the intensity of rays fired from that surface area. As the correct initial intensities are unknown at the start of the calculation the procedure become iterative until correct radiative intensities are resolved.

For the radiative transfer simulation several input parameters are needed. In this case the LES simulation provides the transient data for temperature and species distribution of the medium. The absorption coefficient is calculated from LES data using transient temperature and relevant species distributions. For this the Mixed Gary Gas Model [32] is used in the present study.

The major computational effort in the discrete transfer method is to trace the ray through the cell volumes in the descretised radiation space. An efficient and fast ray calculation algorithm used in our previous studies [30,31] is employed in this work. Although transient calculation of radiation is computationally very expensive the algorithm we use is devised in such way that ray data are calculated only once and stored to re-use in each radiation calculation at every time step with updated temperature and absorption coefficient data.

3. Experimental and computational details

Swirl flames are complicated and resemble flame conditions of many practical combustor devices. Sydney swirl flame experiments provides a high quality experimental data database for the validation computations [33, 34]. From this experimental series flames known as SMH1 and SMH2 are the two flames widely used for validation of combustion simulations in swirl flames. The two flames have the same burner configuration, but different flow conditions. Figure 1 (a) shows the experimental configuration. The SMH1 flame is considered for the present calculations. The burner has a central jet diameter of 3.6mm with a bluff body surrounding it with a diameter of 50mm. The dimensions of the tunnel are 250 x 250 (mm) which covers the burner. A fuel jet consists of CH_4/H_2 (1:1) with an inlet jet velocity (U_j) of 140.8 m/s. The swirl annulus covers the bluff body with an outer diameter of 60mm. As swirl number of 0.32 is maintained for the swirl inlet with an axial (U_s) and tangential (W_s) components of 42.8 m/s and 13.8 m/s respectively. The external ambient co-flow velocity of 20 m/s (U_e) is provided.

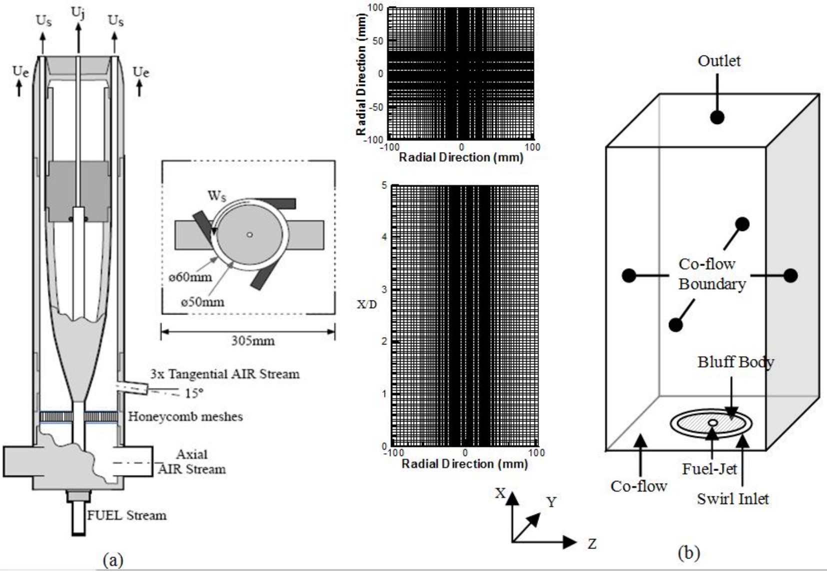

Figure 1 Experimental and computational details of SMH1 flame

The governing differential equations are solved by using the finite volume methodology with an in-house LES code. The computational geometry and grid details are depicted in the Figure 1(b). The computational domain has dimensions of 200 x 200 x 250 (all dimensions are in mm). The axial distance of approximately 70 jet diameters and the burner width of approximately 55 jet diameters is used in order to account the independency of flow entrainment from the surroundings. An inlet jet velocity profile is specified with a $1/7^{th}$ power law profile. Convective outlet boundary condition is used at the outlet surface and all the walls and co-flow boundaries in the domain have been treated as adiabatic. No-slip boundary condition is used in the near wall flow using log-law wall functions. A Cartesian staggered non-uniform grid distribution of 100 x 100 x 100 in the X, Y and Z directions is used to discretise the domain.

4. Results and discussion

The computational time required for the data collection from LES calculations for a time of 20ms is 10 days on a 2.6 GHz Quad core machine with 8 GB memory. The outputs from the LES the temperature, pressure and mole fractions of CO_2 and H_2O are required for the calculation of absorption coefficient and radiation sources in the DT radiation calculation.

Figure 2 - 5 shows typical results from LES. Figure 2 shows the comparison of mean axial velocity with experimental data. It can be seen that agreement is generally very good indicating that LES is a good technique for modelling the swirl configuration considered in this study. Comparison of temperature predictions in Figure 3, CO2 mass fraction in Figure 4 and H_2O mass fraction in Figure 5 show reasonably good agreement with data. Overall LES simulations successfully capture flame properties and important flow features like bluff body recirculation zones and collar like flow features surrounding the central low velocity zone located further downstream from the burner exit in the axial direction. A more comprehensive set of LES results for this flame and for other flames in this series are available in [20,21].

Having established that the LES predictions in this flame are reasonably good and close to experimental measurements transient LES data is used to establish TRI effects in a post processing manner. To compare with RANS type results, where time averaged data is used, here mean LES data is also used to perform separate radiation calculations. By performing radiation calculations with both time averaged data and transient LES data in this case provide a clear indication of the difference one would obtain when averaged temperature and species concentrations are used as opposed to fluctuating temperature and species concentrations for radiation calculations.

For radiation calculations the gas mixture is assumed to be absorbing and emitting medium. Scattering is neglected in the present calculations. All the surfaces are treated as gray and diffuse. The boundaries of the computational domain are assumed to be black bodies at 300 K. The number of rays used is 256 from each boundary surface. In the present DTM code ray intersection data is saved as a file, no ray tracing is required after the first iteration, available ray data can be readily used making the process very efficient. The time taken to generate the ray intersection data file is about 30 minutes and time taken for DTM radiative transfer simulation is only 130 seconds on a 2.6 GHz Quad core machine with 8 GB memory.

Figure 6(a) shows a typical instantaneous temperature field on the central X-Z plane obtained from the LES results and Figure 6(b) shows the time averaged temperature field. Similar contour plots could be shown for CO_2 and H_2O but not presented here in the interest of brevity. First to illustrate the difference between TRI effects we present absorption coefficient and radiative sources at four chosen points in the flame. A typical contour plot of instantaneous radiation source terms on the central X-Z plane obtained from DTM and the locations of some monitoring points are shown in Figure 7. It can be seen that source term distributions clearly reflect the highly turbulent nature of radiation effects. Large variations ranging from -10 to 1700 kW/m^3 indicate that local

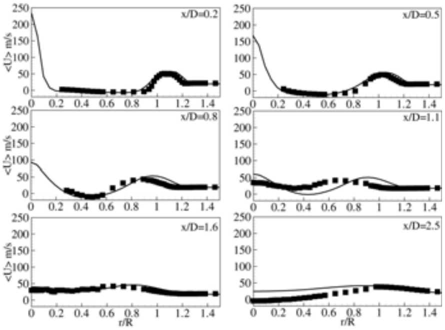

Figure 2 Radial plots of mean swirl velocity (m/s) at different axial locations

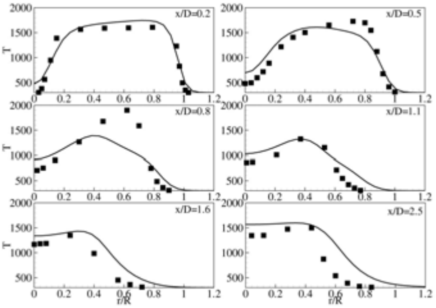

Figure 3 Radial plots of mean temperature (K) at different axial location

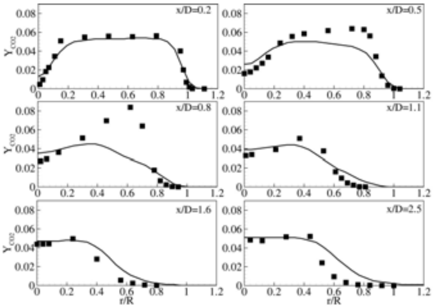

Figure 4 Radial plots of mean mass fraction of CO2 at different axial locations

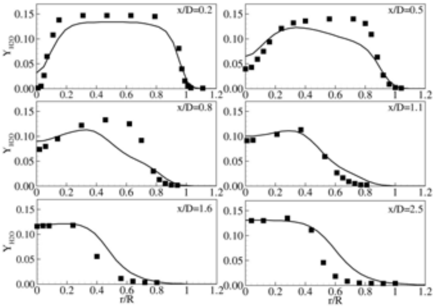

Figure 5 Radial plots of mean mass fraction of H2O at different axial locations

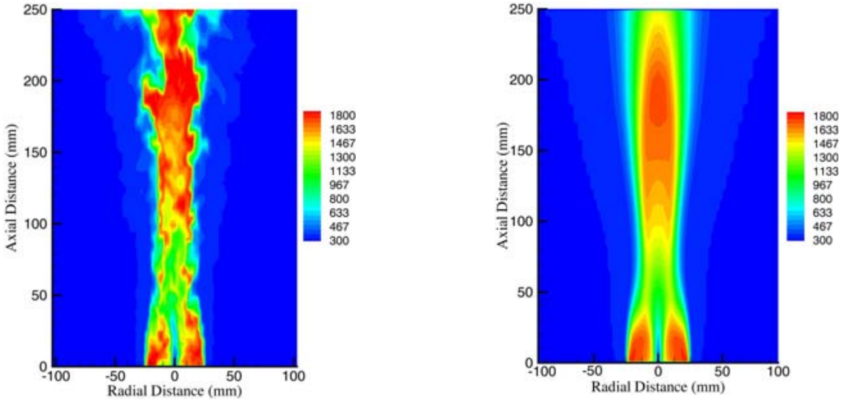

Figure 6 Instantaneous (a) and averaged (b) temperature contours at the centre plane

variations due to turbulent effects are very significant. Figure 8 shows the calculated absorption coefficient at the monitoring locations marked on Figure 7. Also shown by the solid line is the absorption coefficient calculated on the basis of time averaged data. It can be seen that transient absorption coefficient can vary due to TRI effects and the mean value of the transient absorption coefficient shown by the doted straight line is different to the mean value calculated using time averaged data. The difference depends on the turbulence levels (location). At location 3 for example the difference between the mean of the true transient absorption coefficient and that calculated from time averaged properties is 3 %. This location is in the region of the vortex breakdown zone where turbulent fluctuations are considerable. In terms of percentage it appears that temperature and species fluctuations do not significantly contribute to absorption coefficient fluctuations in this case.

Figure 9 shows calculated radiation source terms using time averaged data and instantaneous data at these locations in the flame. It can be seen that depending on the location (fluctuating parameters) radiation source can vary considerably from the value calculated on the basis of time averaged data. Figure 9 (location 3 and 4) for example shows differences of 7.5 % and 17.8 % respectively. These local variations are very significant. Noting that the data set used here is a three-dimensional data set one has to examine differences in many locations to quantify the effect of turbulence fluctuations on radiation. Figure 10 shows the comparison of the sum of the absolute values of radiation source terms for the entire flame obtained from transient calculations and that obtained from the time averaged data. It should be noted that radiation source term can be positive or negative therefore the absolute value is used here. It can be seen that averaged sum of the source term taken from transient calculations is approximately 17% higher than the value calculated from time averaged data. This is very significant. The difference indicates that inclusion of TRI effects results in higher values of radiation source terms. These observations are consistent with the findings of Li and Modest [35]. It should be noted that the present flame considered in not a strongly radiating flame therefore this effect could be much higher in other luminous flames.

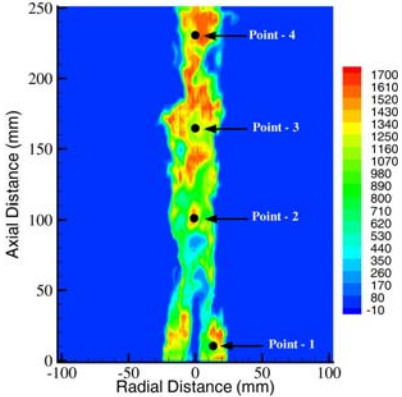

Figure 7 Contours of radiation source (kW/m^3) at the central plane and monitoring locations

Modest et al [17,18] on the basis of DNS type flame calculations have attempted to quantify TRI effects by plotting the temperature self correlation $< T^4 > / < T >^4$. Figure 11 shows a contour plot of the temperature self correlation on the central X-Z plane and Figure 12 shows the temperature self correlation at four line sections of the central plane marked in Figure 13. Both figures indicate that at locations where the flame temperatures are high and the fluctuations are high temperature self correlation can be as high as 4.5 indicating that the TRI effects are very significant.

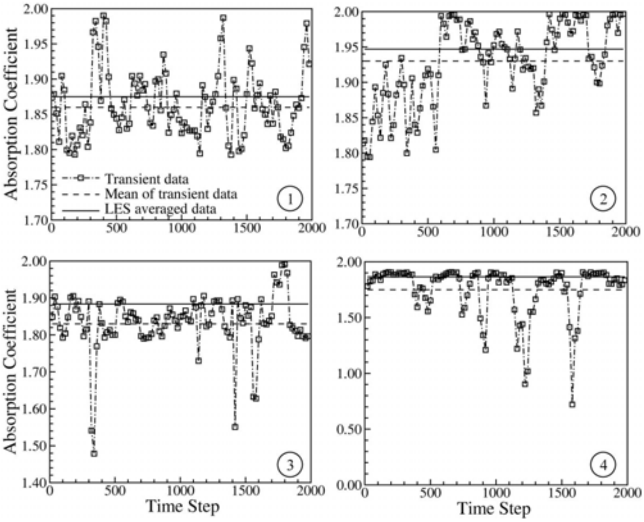

Figure 8 Absorption coefficients at monitoring points

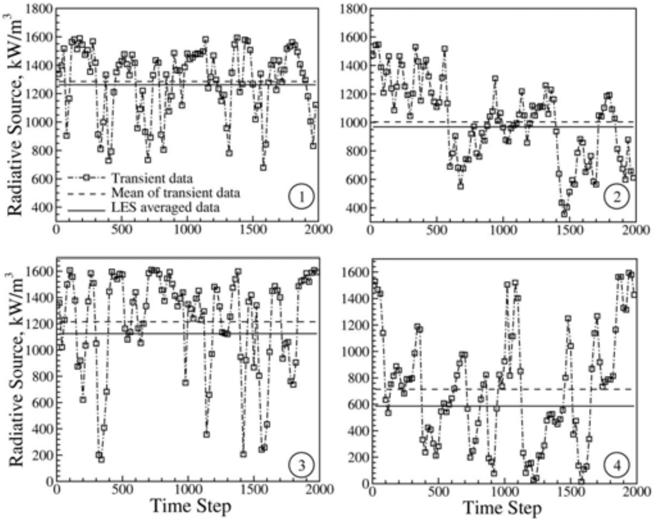

Figure 9 Radiative sources at monitoring points

In general all observations obtained from present DT calculations using LES data indicate that TRI effects are very significant in turbulent flames. Radiation calculation based on time averaged data tend to under estimate radiation source terms and temperature fluctuations plays major role in TRI. Further work to correlate these observations to actual temperature predictions including coupled TRI is underway.

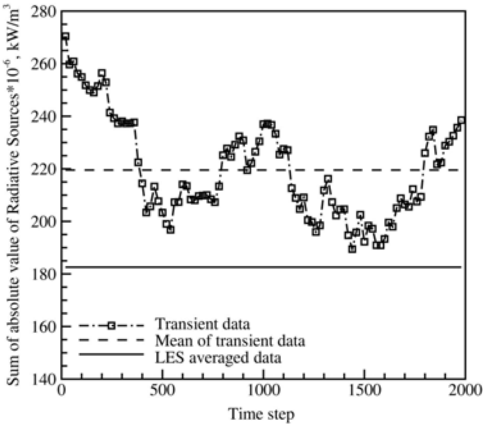

Figure 10 Sum of absolute value of radiative sources

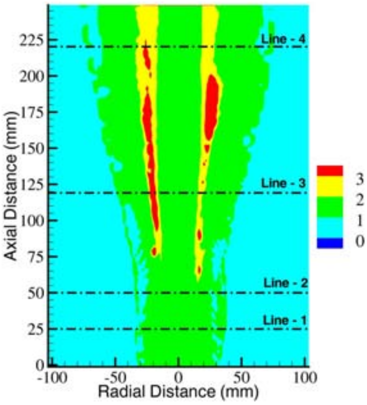

Figure 11 Contours of temperature self correlation $< T^4 > / < T >^4$ at the central plane

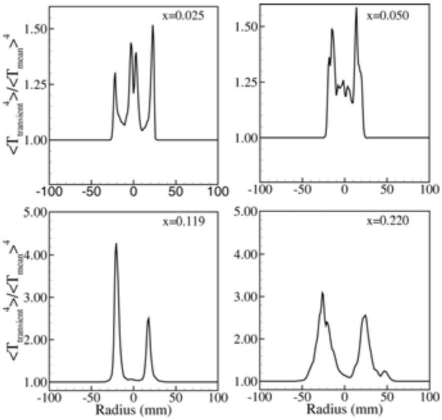

Figure 12 Radial plots of temperature self correlation at different axial locations

5. Conclusions

Using a transient data set from LES this study demonstrate the effects of turbulence/radiation in a swirl flame. The SMH1 swirl flame from the Sydney University experimental database has been considered in these simulations. Radiation calculations using transient data has been performed using the DT method which incorporates the weighted sum of gray gas model for radiation property calculations. For comparison purposes radiation calculations have also been done using time averaged LES data. The results show that there are considerable differences between the values obtained using transient data and those calculated using time averaged data. Temperature self correlation can be as high as 4.5 at certain locations of the flame and contribution of temperature and absorption coefficient fluctuations could result in considerable source term variations when compared to values calculated on the basis of time averaged data. In this study it appears that there is a difference of approximately 17 percent in source term values. It should be emphasised that the present study is an uncoupled radiation calculation and further work to consider full coupling to investigate these effects is underway.

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