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LES Modelling of Air and Oxy-Fuel Pulverised Coal Combustion – Impact on Flame Properties

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Abstract

Large eddy simulations (LES) are used in a CFD model to simulate air- and oxy-fired pulverised coal combustion in a 0.5 MWth combustion test facility. Simulations are carried out using two different burners, namely, a triple staged low-NOx wall fired burner and an IFRF Aerodynamically Air-Staged Burner (AASB). Non-gray radiation is considered in order to deal with the spectral nature of absorption and emission by high levels of combustion products in oxy-fuel combustion. Predictions using LES are compared with Reynolds-Averaged Navier-Stokes (RANS) calculations using variants of the *k*-ε model for turbulence and against available experimental measurements. The results suggest that LES can offer improvements over RANS in predicting recirculation zones and flame properties of the pulverised combustion systems investigated. Flame flickering frequencies from the LES simulations are calculated and validated against available measurements. The work presented demonstrates the potential importance of using LES turbulence models for coal combustion.

Key Words: LES, pulverised coal combustion, oxy-fuel, radiation, flicker

1. Introduction

The introduction of carbon capture and storage (CCS) techniques for both combustion of pulverised coal with air and with oxygen requires increases in plant efficiency. For this purpose computational fluid dynamics (CFD) methods have been used to analyse combustion chamber performance (e.g. [1-3]). Accurate prediction of the particle and velocity distributions are critical for predicting flame characteristics and ultimately heat fluxes in a pulverised fuel (pf) combustion system. In commercial CFD codes, detailed models for combustion, emissions, turbulence and radiative heat transfer are used; however, because of the computational limitations many of the processes are simplified and in particular turbulence-radiation interactions (TRI) [4, 5] are normally neglected. Recent experience in modelling pf coal and co-firing cases by authors [6, 7] emphasised particularly the difficulty of accurate prediction of radiation in a coal-fired furnace due to shortcomings of some of the sub-models.

In this paper, we attempt to accurately predict the radiation to the furnace wall by using large eddy simulation (LES) for pf coal combustion in an air- and oxy-fired combustion test facility (CTF). Modelling the intermittency of coal flames presents a problem when using steady Reynolds-averaged Navier Stokes (RANS) based turbulence models because the flame flicker cannot be calculated due to averaging techniques. LES has been widely applied to turbulent gaseous and spray flames but only a few studies have been reported for pf coal systems [8-11]. In the present study we investigate the impact of LES on the flow, energy and species predictions from various coal and oxy-coal flames and try to explain these through the demonstration of intermittency effects.

2. Numerical Modelling

A commercial CFD program, ANSYS FLUENT© version 12 [12] has been used to model the CTF. This uses an unstructured, co-located, finite volume discretisation to solve the fluid flow equations in computational space. To calculate turbulent combustion using LES, Favre-filtered mass, momentum, energy and species equations [13] are solved in space and time. The standard Smagorinsky model [14] is used to calculate the eddy viscosity and the model constant is calculated using the dynamic Lilly approach in compressible fluids [15]. The use of unsteady RANS (URANS) was considered but initial results suggested no significant improvement in numerical predictions.

The coal combustion model used is similar to that reported in our previous papers [6, 7]. An overall devolatilisation step is used to determine the devolatilisation of the coal particle; the volatile matter consists of the yield of gas and tar. An eddy dissipation model is used for volatile combustion and is used to couple turbulence and chemical reactions in order to calculate the reaction rates. As before, the char combustion sub-model is based on Smith's intrinsic model [16]. The important heterogeneous reactions may be simplified via a global form to:

$$C\text{ (char)} + 0.5\ O_2 = CO \qquad \text{(R1)}$$

$$CO + 0.5\ O_2 = CO_2 \qquad \text{(R2)}$$

In the case of oxy-fuel combustion, high concentrations of CO_2 and H_2O can play a role in char oxidation/gasification. Reactions for soot formation and oxidation [6, 12] and for gasification were not included. Previous work showed no significant impact [17] in incident radiation fluxes for a similar case.

The coal particles are represented by statistical Lagrangian particles which are tracked in the three dimensional time dependent flow field generated by the LES. The trajectories of the particles are calculated by solving the particle momentum equation, and dispersion is accounted for using random Gaussian fluctuations linked to the large eddy time scale [18]. The size distribution of the coal particles is fitted to a Rosin–Rammler distribution ranging from 6 to 325μm based on the experimental data.

Three experimental cases are studied using LES and RANS as shown in Table 1. For RANS modelling, the standard governing equations are used as described in our earlier studies [6, 7]. Turbulence is modelled using the RNG *k*-*ε* model in Case 1 as the flow is dominated by a high swirl component in the secondary and tertiary inlets and the standard *k*-*ε* model is used in Case 2 and Case 3.

The computational grid used is a fully structured hexahedral mesh. The total number of grid cells employed is 1.6million. These are concentrated in the near-burner region where characteristic grid spacing is 1-2mm. In the latter section, characteristic grid spacing normal to the flow is 5-10mm and parallel to the flow 50mm. The time step used for LES is 0.2ms. The grid is sufficient to provide an independent RANS solution however for LES the filter width ($\Delta = V^{1/3}$) may be having significant impact on the results. The expected superiority of LES over RANS depends on a number of parameters including the filter width. However, control over the filter width was limited by available resources. With the grid size and time step employed computational times are 40 hrs per 0.1s flow time, compared to RANS where convergence is achieved in 140 hrs on the same machine[1] when using a gray radiation model.

2.1 Radiation Processes

In industrial pf boilers, radiative heat transfer dominates and an accurate prediction is vital. The RTE, Eq. (1), mathematically describes the transport of radiative intensity through a medium as below:

$$\frac{dI_{\lambda}(\vec{\mathbf{r}},\vec{\mathbf{s}})}{ds} = -(k_{a,\lambda} + \sigma_{s\lambda})I_{\lambda}(\vec{\mathbf{r}},\vec{\mathbf{s}}) + k_{a,\lambda}I_{\lambda,b} + \frac{\sigma_{s\lambda}}{4\pi}\int_{\Omega=0}^{4\pi} I'_{\lambda}(\vec{\mathbf{r}},\vec{\mathbf{s}}')\phi(\vec{\mathbf{s}}.\vec{\mathbf{s}}')d\Omega' \qquad (1)$$

[1] We are using 8 cores, 4GB RAM on a centralised Linux cluster

The intensity $I_\lambda(\vec{\mathbf{r}},\vec{\mathbf{s}})$ at a particular wavelength λ, position $\vec{\mathbf{r}}$ in direction $\vec{\mathbf{s}}$ is attenuated by absorption and scattering as it travels and is augmented by in-scattering and emission from the medium. The properties of the medium such as the absorption coefficient, $k_{a,\lambda}$ and the scattering coefficient, $\sigma_{s\lambda}$ determine the amount of attenuation and are dependent upon the wavelength. The scattering phase function $\phi(\vec{\mathbf{s}}.\vec{\mathbf{s}}')$, provides the directional dependence of the scattering. For air-coal combustion, the radiation may generally be considered to be gray and hence the radiative properties of gases, particles and incident radiation are assumed to be independent of wavelength.

In oxy-fuel coal flames where the CO_2 levels are high, the gas phase emission may be significant. Treating an oxy-fuel coal flame as gray may lead to inaccuracies in the calculation of radiation due to the increased concentrations of CO_2 and H_2O. The combustion products have strong absorption and emission bands caused by transitions between energy levels of CO_2 and H_2O at wavelengths important in combustion and hence exhibit spectral properties that a gray model cannot account for.

For all the cases investigated in the present study, we have used a gray formulation of the weighted sum of gray gases model (WSGGM), coupled with the discrete ordinates method (DOM) [17, 19], to predict the gaseous absorption and emission. The total emissivity is calculated using the WSGGM, and then a gray absorption coefficient is calculated by assuming a mean path length of radiation. For oxy-coal combustion, in addition to the gray model, a spectral model, the full spectrum k-distribution (FSK) method [20] for the gas properties has also been used [21-22]. This model was implemented in order to demonstrate the impact of the gas radiative properties on the results. Particulate properties are assumed to be gray. The sensitivity of the predicted radiative heat fluxes to the radiative properties of the particles is not neglectable; however, we have not performed a sensitivity analysis here. Values previously adopted for the particle emissivities [6, 7] were used although there is still some uncertainty about their choice [23].

Since the heat transfer in the present case is largely dominated by radiation and the fluctuations in density and temperature are inextricably coupled, TRI may be the best option. TRI has been coupled with RANS turbulence models for combusting cases [5] and has shown significant impact on the solution. However, TRI in LES is computationally expensive and this is compounded by the size of furnace considered here. In the present LES simulations, radiation is treated without any sub grid scale (SGS) models to account for the effects of SGS radiation fluxes on resolved scales.

3. Experimental Cases Considered

Three test cases were chosen based on published experimental data obtained using the RWE npower 0.5 MWth CTF at Didcot Power station, UK [7, 24-27]. The dimensions and details of the CTF are given in [26, 27] but essentially it consists of a 0.8m square ceramic lined furnace approximately 4m long followed by a convergent section leading to a simulated economiser region. Table 1 gives the experimental conditions. Both coals A and B have similar properties and are typical bituminous power station coals. Measurements taken include surface incidence radiation along the vertical chamber walls, flame photographs and, for Cases 2 and 3, flame and the furnace exit temperatures and flame oscillation frequency determined photometrically. Data was also available on NOx and unburned carbon in ash for Case 1. The measurement techniques and data have been reported previously in [7, 24, 25].

Two different burners were used for the tests. The characteristics of these burners differ greatly. The Doosan-Babcock triple-staged low-NOx burner is scaled based on total residence time in the furnace. The IFRF AASB burner is scaled based on constant velocities. The IFRF burner provides a higher intensity flame with greater stability limits due to inlet velocities at least one magnitude greater than those of the Doosan-Babcock burner. Burner details can be found in [26, 27].

The coal properties and inlet conditions considered for each case are given in Table 2 and Table 3, respectively. Case 1 has previously been extensively studied by us [7], using variants of the *k*-*ε* RANS turbulence model; however we were unable to reproduce the measured wall fluxes to a sufficient degree of accuracy. Hence we now compare the previous predictions to LES case. Cases 2 and 3 are part of a recent experimental programme looking at heat transfer from oxy-fuel flames [19, 24].

4. Results and Discussion

Figure 1a presents axial velocity distribution in the domain for the three cases investigated using RANS and LES. We have shown instantaneous LES fields in order to demonstrate intermittent effects. The axial velocity distribution predicted by LES indicates stronger recirculation zones than RANS simulations in all cases. Figure 2 compares the time-averaged axial velocity and temperature contours for Case 2. The average internal recirculation zone strength is higher in the LES case.

Figure 1b presents temperature contours with superimposed velocity vectors for the three experimental cases considered. The LES calculation shows some flame on the inner diameter of the center-body (secondary and tertiary passage exit), while the RANS calculation does not. Predicted magnitude of the secondary (and tertiary for Case 1) velocity vectors by LES is greater than when using RANS models. In general, LES is shown to predict swirl dominated flows more accurately than RANS [28].

Figure 3 presents a comparison of the (time-averaged) wall surface incident radiation fluxes from RANS and LES against measurements. In the case of RANS the predictions are extracted from converged solutions. In the case of LES, the simulations were performed for a sufficiently long period of time to obtain a statistically consistent numerical solution. For instance in Case 1, the sampling frequency was 0.6 ms and sampling was carried out for 0.5s after 5.5s of flow time. None of the curves gives a perfect match to the experimental data. Apart from the turbulence approach this is also due to the simplicity of the other physical sub-models used, in particular the gray gas and particles radiation model, reduced chemistry, and averaging practises. In Cases 2 and 3 we had difficulty in reproducing the observed incident radiation measurements. Dissociation effects are neglected; in the more intense flames obtained with the IFRF burner dissociation may play an important part in reducing temperatures in the flame region. As temperature and radiation are intrinsically linked, this would also reduce the radiative heat fluxes. There are significant differences between the RANS and the LES predictions in the near-burner region in all cases. RANS using a spectral gas radiation model captures the surface incident radiation more accurately than using the gray model for the oxy-coal combustion case. Hence in order to apply LES successfully to oxy-coal combustion integration of a spectral gas radiation model is required.

Table 4 shows the predicted and measured furnace exit gas temperatures. For air-firing, RANS simulations under predict exit temperatures by up to 120K. For the oxy-coal case, RANS appears to predict the exit temperature well, however it should be noted that the associated radiation fluxes have higher errors in the oxy-coal cases assuming gray gas radiation and in fact heat transfer is expected to be less well predicted mostly due to the radiation issues discussed earlier. Hence correct exit temperature does not necessarily suggest correct model predictions. LES predicts increased exit temperatures in the air-firing cases; for both Case 1 and Case 2, closer to the experimental measurements. For the oxy-coal case the exit temperature is actually reduced by the use of LES which again is closer to the experimental measurements.

Figure 4 demonstrates the importance of flame intermittency in the calculation of radiation loss from turbulent semi-opaque flames. As can be seen from the image, in the RANS cases the temperature at the flame edge has a smooth average value whereas in LES, the flame edge is characterised by hot regions which are much hotter and hence much higher-emitting than the surrounding flame. These hot regions are caused by large eddies of hot gas fully resolved in the LES calculations, which are converted from the centre of the flame to the edges and thus contribute significantly to radiation loss from the flame. Smith [29] addressed this problem by assuming sinusoidal flame-edge temperature fluctuations and showed that predicted lateral radiation emitted from the flame can be greatly increased compared to assuming an average flame-edge temperature. This effect can be seen in Fig. 3, as in the region of the flame the incident radiation is increased at the walls.

The flame oscillation frequency is numerically calculated in the present study. Unlike in premixed and non-premixed flames, the flame length, volume or surface is not clearly defined in the case of pf coal combustion. This is mainly due to the treatment of the coal particles. The flame flickering frequency has been calculated following the experimental procedure used [30] in the same CTF. Figure 5 illustrates the region of interest by superimposing the LES image on a typical experimental video image. The location of the flame surface is defined by local air-fuel ratio. Incident radiation signal on the flame surface is collected within the root and middle regions of the flame. In order to calculate the flicker frequency, we used the power-density-weighted approach within the entire frequency range. More details of the methodology can be found in [30, 31]. Application of the FFT on numerical signal generates the normalised power spectral density (PSD) as shown in Fig. 6. The frequency spectrum of a flicker signal is identified to have various frequency components due to the reasons outlined in [31]. More specifically, in coal flames multiple frequencies are expected due to the combined effect of laminar and turbulent time scales.

Based on the PSD approach, the flicker frequency of the root and middle region for Case 1 is calculated as 17 and 13 Hz, respectively. In Case 2 the flicker frequency within the root region is calculated as 12 Hz. In Case 3, it is calculated to be 14.5 and 8 Hz in comparison to experiments of 10.5 and 7 Hz [25], which is in reasonable agreement. However, the accuracy of the 'flicker frequency' from numerical simulations is found to be dependent on the flame length and the surface chosen.

The presence of large incompletely combusted eddies in the flame gases can have a significant effect on emissions of unburned carbon, NO, CO and unburned hydrocarbon gases. In particular CO concentrations can be greatly above equilibrium values in pulverised coal flames [32]. In Case 1, LES and RANS have predicted the unburned carbon as 1.0 % and 1.35 % against experimental measurements of 3.0%. The predictions of NO from LES and RANS are found to be 316 and 300 ppm dry against measurements of 325ppm dry. However, predictions of CO by LES and RANS are found to be 110 and 150 ppm dry respectively against 20 ppm dry of measured values. Improvements in the prediction of the CO concentration would require a more detailed combustion model.

5. Conclusions

In this investigation, LES simulations of radiative heat transfer from air and oxy-fired pulverised coal combustions in a 0.5 MWth furnace have been performed. The key findings are as follows:

LES can be used to study the instantaneous flow features of coal flames such as turbulence interactions with the flame and the recirculation zones, which are important for flame stability.

LES predictions of surface incident radiation differ significantly from RANS in all three cases. In particular, lateral radiation in the near-burner section is enhanced with LES. It is believed this is due to the ability of the LES to capture intermittency effects of the coal flame. For oxy-coal combustion, we have demonstrated the importance of the gas radiative properties.

Numerical flame oscillation frequencies have been calculated using the time history of the surface incident radiation, which compare well to experimental measurements.

The impact of the presence of large eddies on emissions of CO is highlighted. This confirms the pressing need to develop more rigorous methods of accounting for the intermittency of CO and NOx in exhaust gases.

LES of coal combustion requires substantial computational resources. The development of more efficient LES codes which can handle heterogeneous combustion is hence desirable, as to further refine our grid would render computational requirements prohibitive.

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LES Modelling of Air and Oxy-Fuel Pulverised Coal Combustion - Impact on Flame Properties

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Tables

Table 1

Test cases considered for LES simulations

	Burner Type	Firing Type	Coal	% Excess Oxygen
Case 1	Triple Stage–Low NOx Burner	Air	Coal A	3.0
Case 2	IFRF	Air	Coal B	3.0
Case 3	IFRF	Oxy-Fuel	Coal B	3.0

Table 2
Coal Properties (wt% as received)

	Coal A	Coal B
Inherent Moisture %	4.00	4.23
Ash %	17.74	13.59
VM %	27.48	29.8
FC %	50.78	52.38
C %	63.99	66.41
H %	4.210	4.64
N %	1.360	1.91
S %	1.112	0.38
GCV MJ/kg	26.47	27.39

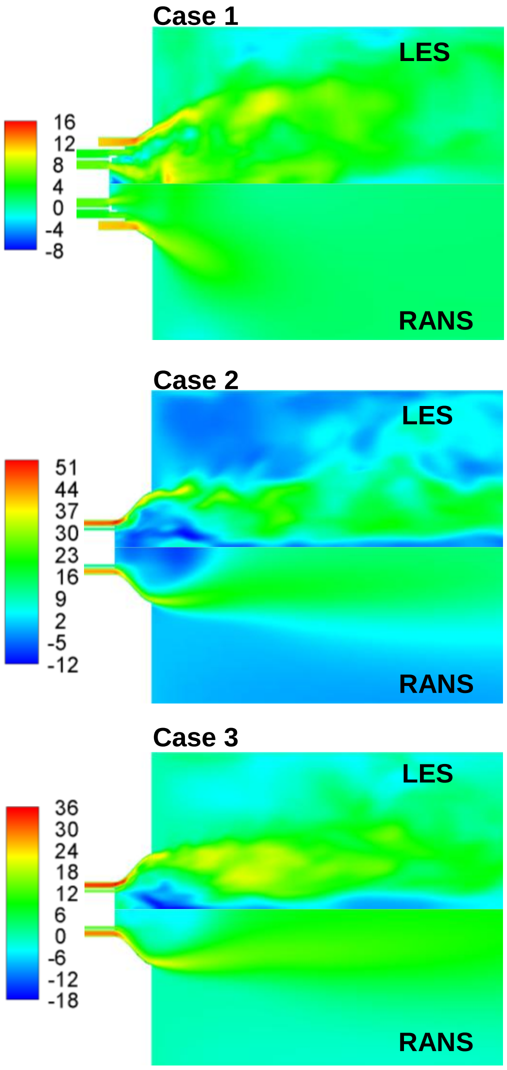
Table 3
Burner Flow Rates

	Primary Inlet (kg/h)	Secondary Inlet (kg/h)	Tertiary Inlet (kg/h)	Mass flow rate of coal (kg/h)	Oxidant
Case 1	156.96	118.08	419.04	65.33	Air
Case 2	110	620	-	68	Air
Case 3	155	600	-	68	$O_2 + CO_2$

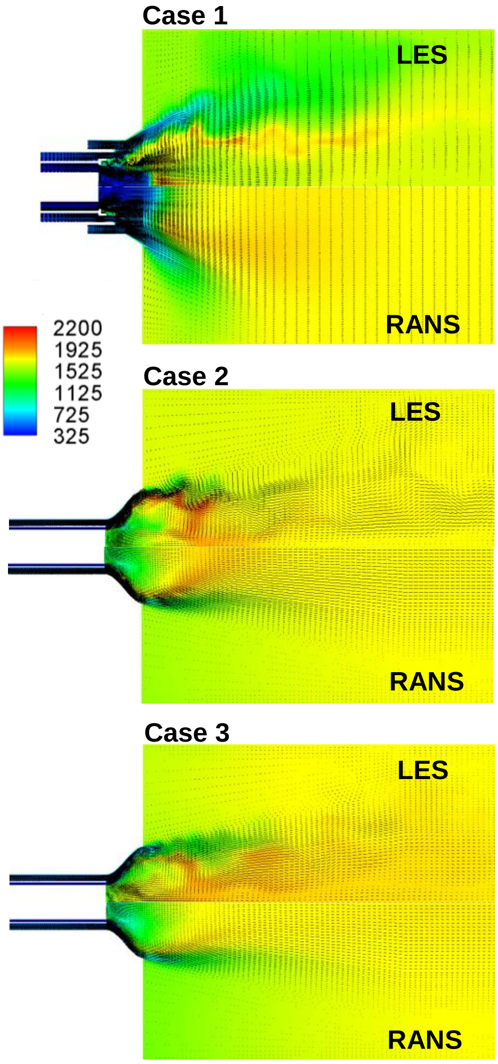
Table 4
Exit temperatures of the CTF (K).

	RANS	**LES**	**Measurements**
Case 1	1479	1564	1597 ± 25
Case 2	1367	1417	1450 ± 25
Case 3	1465	1454	1425 ± 25

Figures

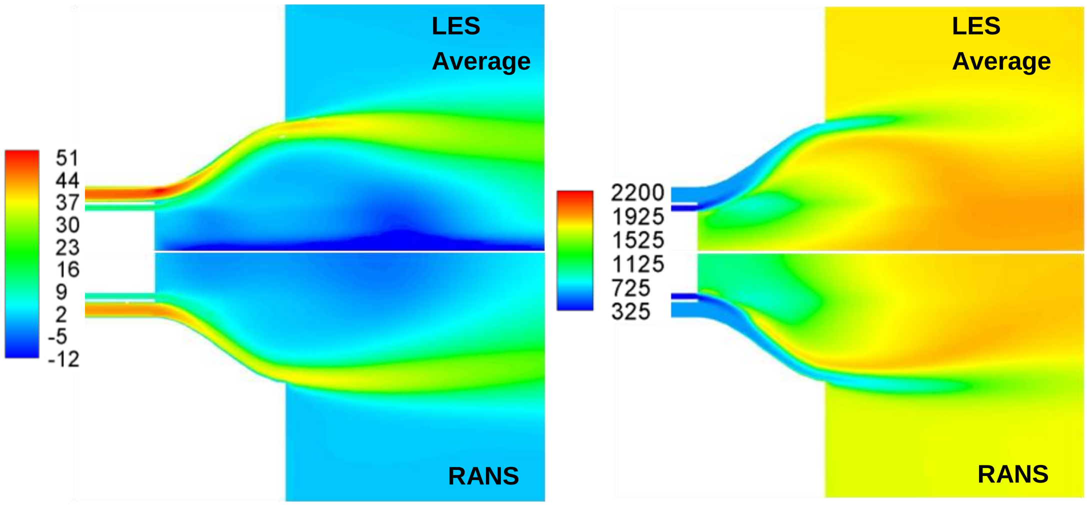


(a)



(b)

Fig.1a. Axial velocity distributions from LES and RANS. Individual axial velocity legend is shown in m/s. 1b. Velocity vectors are superimposed over temperature distribution from LES and RANS. Temperature legend is shown in ^{o}K.



(a) (b)

Fig. 2. Comparison of time-averaged contours from LES against RANS for Case 2. (a) Axial velocity in m/s. (b) Temperature in ^{o}K.

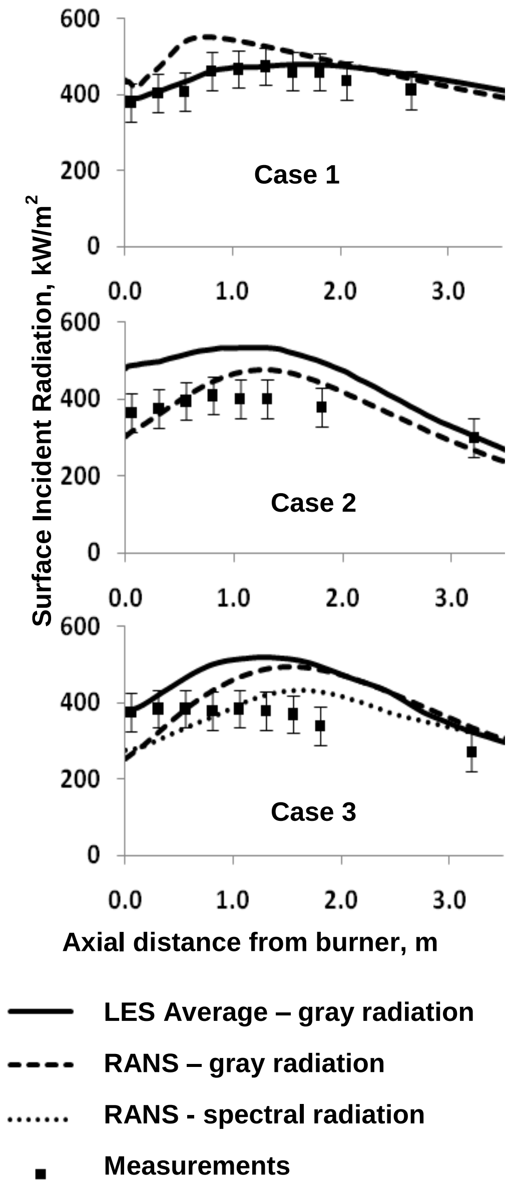


Fig.3. Numerical predictions of surface incident radiation along furnace wall centreline in the direction of flow from the burner exit using RANS and LES compared to experimental measurements.

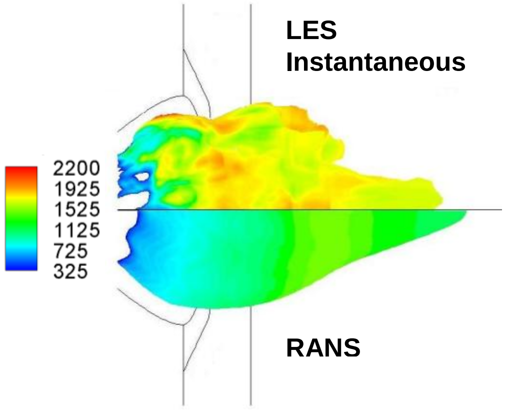


Fig.4. Flame volume for the IFRF air-coal flame (Case 2) coloured by temperature in ^{o}K.

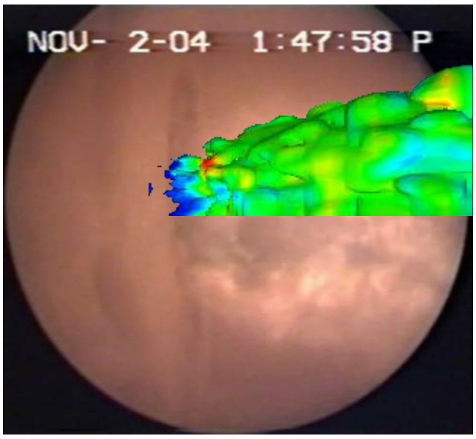


Fig.5. Calculated incident radiation from LES of the pulverised air-coal flame (Case 1) is superimposed on a typical coal flame video image, showing the region of interest to determine the flame frequency.

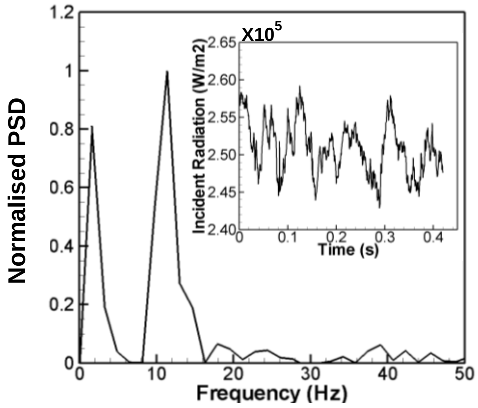


Fig.6. Normalised power spectral density from the root region of the flame (Case 1). Corresponding incident radiation signal against time is shown in inset.

Figure Captions

Fig.1a. Axial velocity distributions from LES and RANS. Individual axial velocity legend is shown in m/s. 1b. Velocity vectors are superimposed over temperature distribution from LES and RANS. Temperature legend is shown in ^{o}K.

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Fig.4. Flame volume for the IFRF air-coal flame (Case 2) coloured by temperature in ^{o}K.

Fig.5. Calculated incident radiation from LES of the pulverised air-coal flame (Case 1) is superimposed on a typical coal flame video image, showing the region of interest to determine the flame frequency.

Fig.6. Normalised power spectral density from the root region of the flame (Case 1). Corresponding incident radiation signal against time is shown in inset.