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Leeds University

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Co-firing Coal/Biomass and the Estimation of Burnout and NOx Formation

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Executive Summary

Co-firing of coal and biomass is widely used in the UK, Europe and the US and is now largely routine at least up to 20% biomass on a thermal basis. There are still problems associated with the use of biomass, for example, often after grinding the biomass some particles may be larger than pulverised coal and this can result in enhanced carbon in ash. Whilst this problem can be minimised an understanding of the combustion of the larger particles is useful. An additional issue is that biomass contains a considerable amount of potassium which is easily released and can cause deposits and corrosion on boiler tubes. Finally although biomass usually contains less fuel-N than coal the detailed mechanism of NO release from biomass is not well known and a better understanding might make possible the reduction of these levels.

The aim of this project is thus to improve the level of understanding of the underpinning science for the co-firing of coal and biomass in utility boilers. This project is concerned with a modelling study of the co-firing of coal and biomass, up to 20% thermal of the total input. The project is particularly directed towards those biomass materials that form large, irregular particles that do not burnout readily, and in predicting the formation of NOx.

After some consideration it was decided that a computer modelling investigation would be undertaken of cofiring coal and biomass in an industrial combustion test facility, the CTF at RWE npower at Didcot. This had rating of 0.5 MW and was fitted with a Doosan Babcock (Mitsui Babcock) Mark III burner. This had the advantage that a considerable number of experimental results had been obtained using this combustion test facility for a wide range of coals and coal/biomass blends. Three single coals and five coal/biomass mixtures were selected by RWE npower for the project and data for them was made available. In addition, results have been computed for a torrefied wood. This was not part of the original proposal but in view of the interest in this material this case was examined although no experimental results are available at this time. A second decision was to use a commercial code Fluent, version 6.

In typical co-firing of coal and biomass the combustion of the coal itself is the major component of the flame and an accurate mechanism for this part of the overall combustion is necessary. Fluent contains a default coal combustion mechanism including flow and heat transfer steps and aspects of that code can be modified by the user, and this was done during the project. Therefore in the first stage of the project particular attention has been paid to the combustion of a single coal, Gascoigne Wood, where a substantial amount of data is available.

For the first step of coal combustion, namely devolatilisation we have previously used the network devolatilisation code FG-DVC and we decided to use that in this project. By comparison with other similar coals a rate expression was derived. This has a high value compared with many such expressions obtained by small scale laboratory experiments and this has a major significance on the rate of volatile release which influences flame holding and near-burner flame shape. Since the rate is fast it implies that the rate heating-up of the particle plays an important role and so does the correct choice of the specific heat. Likewise the volatiles yield was determined and compared with experimental data and values obtained by using rapidly heated wire mesh experiments. The char burnout model and NOx model were ones used previously with some success.

The case computed was for the combustion with 4% oxygen in the flue gas and the results obtained for flame shape, flame temperature, radiation to the furnace walls, exit gas temperature, unburned carbon in ash and NOx. Different turbulence models a

were tested as was the effect of different soot models on the incident radiation flux. Comparisons were made of the flame shape against experimental video measurements. In addition the computed data was compared against experimentally determined flame temperatures for similar flames available in the literature. Good agreement was obtained except for the radiation measurements for reasons which are still uncertain at the present time. But it is probably related to variation in emissivity as the black coal particle is converted into an ash which has a low emissivity. Whilst the question of the emissivity of the coal char/ash seemed to have been resolved years ago this does not seem to be the case and recent studies have reopened the debate.

A number of coal biomass blends were examined, namely
1. South African coal /milled wood (20% thermal),
2. Russian /Palm Kernel expeller (15% thermal),
3. South African/Miscanthus Giganteus (20% thermal),
4. South African /Olive waste (15% thermal).

The reaction data and volatile yields for the additional coals, South African and Russian, were obtained in the same way as for Gascoigne Wood coal.

The biomass particles were examined by SEM. It was clear that the milled wood and the miscanthus contained large particles whilst the PKE and the Olive waste did not (although with particles which are slightly larger than the coal). This information was used in the combustion models.

The effect of the large biomass particles has an effect of the choice of the biomass models, the heating-up equations, devolatilisation and burning rates particularly. The effect of moisture on the biomass particles was examined. Computed heating-up equations were obtained for two particle sizes and different heating conditions up to 10% moisture, and less accurately up to 50% moisture.

The devolatilisation rate and yields were estimated via the bio-FG model, and in the case of the former the value is again a higher values. If this conclusion is correct this implies the importance of the factors controlling the heating-up rate, the accuracy of the specific heat data and the effect of moisture. The effect of the Biot number is important. Large articles were approximated by an equivalent sphere for both aerodynamic and heating up equations. The reaction rates of large particles could also be approximated in this way but it is not a good approximation for burn-out. Studies of suspended single particles were made using still and video photography to check the models used.

The calculation of furnace exit temperatures, unburned carbon in ash were made and compared against experimental results for all the blends and single coals. Values were also calculated of NOx. For the calculations involving a biomass an allowance was made for the presence of proteins and amino acids in the biomass.

The level of agreement for all these results is discussed and the way in which this can be incorporated into industrial models identified.

In general the level of agreement is good although the model could be improved by using a better heat transfer model incorporating a variable emissivity as the reaction progresses. Better data on the emissivity of the slag at high temperatures would be advantageous. Computation of these flames could be improved by using a more powerful computer so that the coal combustion model could utilise a more detailed coal combustion model which is available. Such models exist but can only be used in conjunction with a zone model because of the complexity of using it with a full CFD model, but industry models could use the more detailed model at the present time.

1. Introduction

Co-firing of coal and biomass is widely used in the UK, Europe and the US and is now largely routine at least up to 20% biomass on a thermal basis. There are still problems associated with the use of biomass, for example, often after grinding the biomass some particles may be larger than pulverised coal and this can result in enhanced carbon in ash. Whilst this problem can be minimised an understanding of the combustion of the larger particles is useful. An additional issue is that biomass contains a considerable amount of potassium which is easily released and can cause deposits and corrosion on boiler tubes. Finally although biomass usually contains less fuel-N than coal the detailed mechanism of NO release from biomass is not well known and a better understanding might make possible the reduction of these levels. The aim of this project is thus to improve the level of understanding of the underpinning science for the co-firing of coal and biomass in utility boilers. This project is concerned with a modelling study of the co-firing of coal and biomass, up to 25% thermal of the total input. The project is particularly directed towards those biomass materials that form large, irregular particles that do not burnout readily, and in predicting the formation of NOx. The specific objectives of this project were:

i) To design sub-models to accurately describe the release of water and volatiles,
ii) To develop understanding of the heat and mass transfer associated with devolatilisation and char combustion in irregular shaped biomass particles,
iii) To test the robustness of these models using laboratory experimental data,
iv) To use the approaches developed above in CFD models for the co-firing of biomass and coal, and to test these models against experimental data available from an industrial Combustion Test Facility.
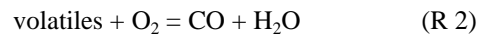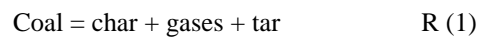
2. Experimental Methodology

In the preliminary discussions with the Industrial Supervisor and with RWE npower it was concluded that the best approach to the project was to use experimental data available from RWE npower for their Combustion Test Facility. This decision effectively determined the systems studied which are given below. It was decided that the Gascoigne Wood data would be used to test the model and then the binary coal-biomass fuels would be investigated.

1. Gascoigne Wood coal-this is used as a standard because it has been widely studied on the CTF and included measurements of flame radiation.
2. Russian coal, which is used as one of the blending coals,
3. South African Coal, which is used as one of the blending coals,
4. South African /milled wood (20% thermal),
5. Russian /Palm Kernel expeller (15% thermal),
6. South African/Miscanthus Giganteus (20% thermal),
7. South African /Olive waste (15% thermal).

In addition the combustion of a blend of South African Coal with torrefied wood (20% thermal) has been investigated using a CFD model, although no experimental data is available for this case. In all the experiments considered here the oxygen content of the flue gases was 4% (dry).

Information was provided by RWE npower (Dr P Stephenson and Dr M Whitehouse) on the construction of the furnace and the burner and these details are given in Appendix 1. The burner is a 0.5 MW rated Doosan Babcock Mark III burner mounted in a rectangular furnace and replicates a burner in a third row of a wall-fired power station.

The CFD model used is the Fluent Version 6 coal combustion model to compute the combustion of coal or coal/biomass blends with Fluent's User Defined Function capability. NOx was computed using the associated Fluent post-processor package. Most details of the use of that model have been previously published for the combustion of pulverized coal [1-4], for co-firing [5] and with biomass alone [6, 7]. Some of the important computational details are given in these references and associated Reports [8, 9] and are briefly summarized an Appendix 2. Some aspects of the User Defined Functions developed in the project are considered later. A key issue is that most calculations we used the two step mechanism

$$Coal = char + gases + tar \qquad R\ (1)$$

$$volatiles + O_2 = CO + H_2O \qquad (R\ 2)$$

$$CO + 0.5\ O_2 = CO_2 \qquad (R\ 3)$$

$$C\ (char) + O_2 = CO \qquad (R\ 4)$$

$$CO + O_2 = CO_2 \qquad (R\ 5)$$

All the computational work was undertaken by Dr L Ma, a Senior Research Fellow who is a member of the Centre for Computational Fluid Dynamics at Leeds University.

In order to meet the stated objectives of the Project the following main studies were made: (1) The nature and properties of the coal and biomass and their rates of decomposition and products, (2) Water evaporation, (3), Turbulence and radiation models, (5) NO prediction program, and (6) Application of the CFD model to the Combustion Test Facility.

2.1 The Nature and Properties of the Coal and Biomass Materials

(a). Composition of the Coals and Biomass.

The compositions of the coal and the biomass materials were given by RWE npower and are listed in Appendix 3. Data for other coals was that used by in recent projects [1-8]. The values for the torrefied wood were based on data taken from reference 9. The data in Appendix 3 are presented in an 'as received form' and were used to derive the quantities required by FG-DVC and the Fluent program.

In order to demonstrate the properties of the fuels in relation to other commonly used fuels they are plotted on a van Krevelen plot below with the exception of the torrefied wood. The properties of this lie in an intermediate poison between coal and biomass.

Figure 1. The van Krevelen Diagram for Biomass and Coal
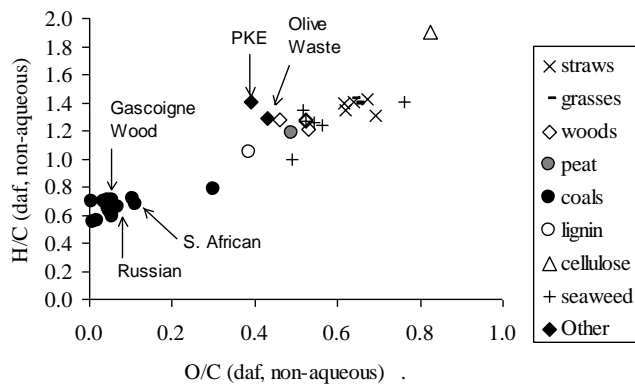
(b) Particle Sizes of the Coals and Biomass.

The particle sizes for the coals were provided by RWE npower. The milled biomass samples vary considerably depending on the type of biomass. In the present experiments the moisture content was lowered by air drying and milling was undertaken to replicate typical sizes found in a power plant. The samples of milled miscanthus, olive waste, wood and PKE provided were examined by electron microscopy at Leeds University, and these are shown below.
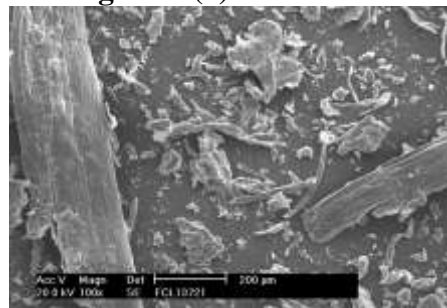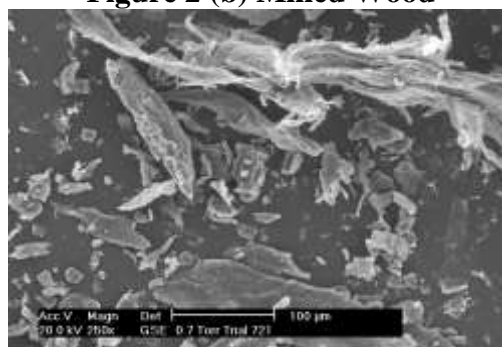
Figure 2 (a) Miscanthus

Figure 2 (b) Milled Wood
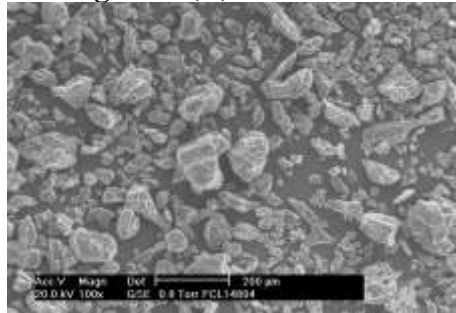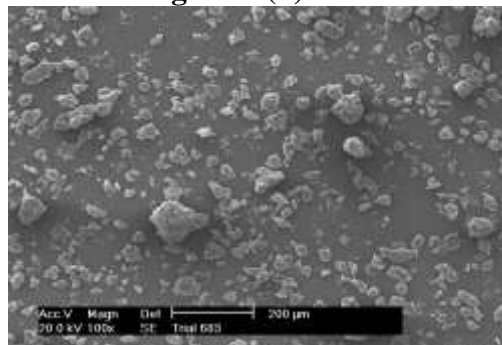
Figure 2 (c) Olive Waste

Figure 2 (d) PKE

The sizes and shapes of the milled Miscanthus particles are very similar to the milled wood (Pine) because they are both fibrous materials. The Olive waste is very similar to the Palm kernel because they are both nut-like materials, although in both cases there are slight variations in the particle sizes. The mixtures of biomass and the coals present complex issues in the definition of the size distribution inputted in to the CFD model. These size distributions can however be handled adequately by the CFD model but there is an issue about the larger sizes of the wood and Miscanthus which will be discussed later.

The figure below shows the distribution in a mixture of South African coal and 15% Olive waste. It consists of a large number of smaller particles with about 5% above 150 μm. The presence of larger irregular sized biomass particles has implication for both their reactivity and their aerodynamic behaviour, and are discussed later.

Figure 3. Blend of South African coal and 15% Olive waste.
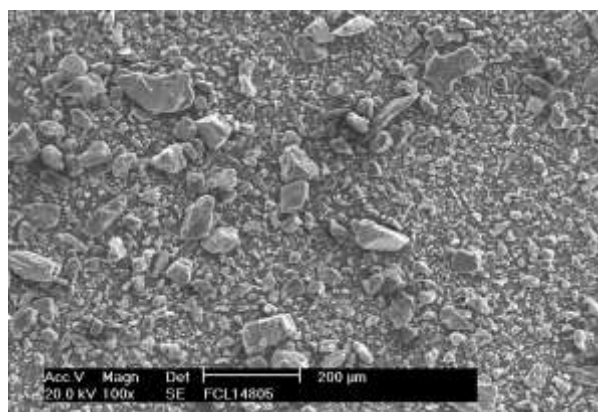
2.2 The Rates and Yields of the Coal and Biomass Decomposition Products

In the case of the coals, the values for devolatilisation rate constants A_d and E_d, for the overall first order step obtained from previous studies on devolatilisation network codes were used. The devolatilisation rate constant parameters for the release of tar, gas and total volatiles for the four coals calculated by FG-DVC [11] and values taken from our previous studies [2, 4, 8] are given in the Table 1 below.

On average for these coals, for the process of overall devolatilisation, this leads to an activation energy, E, of 230 kJ mol^{-1} and a pre-exponential factor, A, of 4.2. 10^{14}. The test coals used in the present studies are similar in nature to those in Table 1 as indicated by their close proximity in Figure 1, and consequently the above value was used for all the coals in this study. This curve is plotted in Appendix 4.

Table 1. Reaction Rate Parameters for Tar, Gas and Total Volatiles, [2, 4, 8].

| Coal (Origin) | Devolatilisation Rates – FG-DVC computed | | | | | |
| | Activation Energy, E_d (J kmol^{-1}) | | | Pre-exponential factor, A_d (s^{-1}) | | |
	Tar	Gas	Total	Tar	Gas	Total
Thoresby	3.3×10^8	2.4×10^8	2.4×10^8	3.8×10^{14}	4.6×10^{13}	5.2×10^{14}
Asfordby	2.0×10^8	2.1×10^8	2.3×10^8	3.7×10^{14}	4.2×10^{13}	4.8×10^{14}
Betts Lane	2.5×10^8	2.3×10^8	2.4×10^8	2.1×10^{14}	3.2×10^{12}	3.3×10^{14}
Pittsburgh#8	2.3×10^8	2.2×10^8	2.3×10^8	3.7×10^{14}	4.8×10^{12}	3.8×10^{14}
Ensham	2.4×10^8	2.7×10^8	2.4×10^8	4.1×10^{14}	3.2×10^{14}	4.3×10^{14}
Prodeco	2.3×10^8	2.4×10^8	2.4×10^8	3.0×10^{14}	4.6×10^{13}	5.2×10^{14}

Experimental devolatilisation rate data can be analysed in a number of ways so that there can be compensation between values of A and E. In the literature there are effectively choices between pairs of high activation energy and high pre-exponential factors or pairs of low values for E and A. The former are obtained by the network codes (FG-DVC, CPD or FLASHCHAIN) or by high temperature studies with high heating rates, the latter constants often from TGA where inadequate data analysis is made. The different sets of kinetics are demonstrated in Appendix 4 where the lower open flame and drop tube data are shown and the wire mesh and TGA results tend to have lower activation energies and would lie across the plot at an angle of 45°. We have found that the choice of one set or the other does not lead to large differences in an overall computation but it does slightly change the location of the flame front in a CFD computation. The choice of 'fast kinetics' is in accordance with our previous conclusions [3], and there is now a substantial body of evidence to support this approach, eg. [12]. This is because in flames the reaction rate is effectively controlled by the heating-up rate that in turn brings in other difficult to define parameters such as water evaporation (small in these experiments) and specific heats where there is still debate about the values of molten coal particles.

Knowledge of the amount of char produced from devolatilisation is an important factor because it plays an important role in determining the amount of unburned carbon in the ash. The reaction conditions at which this devolatilisation takes place is therefore an important issue. On the basis of our earlier studies [2] these are taken to be 10^5 K/s to a temperature of 1773 K in 150ms, which are typical flame conditions.

The yields of volatiles (char is the remainder) for the coals were calculated by FG-DVC using the coal composition and the above conditions and these are given below in Table 2. This approach is significantly different to the experimental method used by Gibbins and co-workers who have used higher temperatures and longer residence times with an electrically heated wire mesh [13, 14]. Using this method the ratio of the high temperature VM to the laboratory value is typically 1.3 to 1.6, and values calculated on this basis are given in bold in Table 2. But these higher values are not really appropriate because the coal particles ignite after 150 ms and burn in the heterogeneous char combustion mode. Notwithstanding that, the agreement between the two methods (columns 2 and 3 is quite good) with the exception of the Russian coal with the high volatile content).

Table 2. Volatile Yields (%wt, daf) for the Coals Studied in the Project

Coal	VM (daf)	Calculated, FG-DVC	Value given by RWE npower	Experimental values
Gascoigne Wood	35.11	55.1	55.47 (a)	48.7 (b)
Russian	43.43	58.1	57.5-69.5	58.3
South African	37.64	54.75	48.9-60.2	49.92

(a) Provided by Dr P Stephenson, (b) CRE data at 1350° C [15]

The reaction rates of biomass these have been widely studied using TGA or drop tube reactors, but there is little direct experimental information on their behaviour in furnace flames where the heating-up rate is important. A first order kinetic rate model has been widely used for all biomass materials. Because of the uncertainty about their high temperaure rate constants we have used values of A= 6×10^{13}₃ 1/s and E = 2.5×10^{8} J/kgmol. The values are based on values previously used for the pf wood combustion and are calculated based on the bio-FG network program [5]. However in this study we have used a single value for all biomass materials including torrefied wood. The values used for biomass and for coal are shown in the figure in Appendix 4.

In the devolatisation model particles are assumed to be spherical and of such a size that the temperature is uniform across the particle, ie thermally thin. The kinetic expression rate for the biomass (and the coals) is only applicable to particles that are thermally thin, and it is clear from the electron micrographs that some biomass particles may fall outside that category. Whether this happens is determined by the Biot Number [16], which can be based on the surface area to volume ratio. It can be concluded that the thermally thin regime can be defined as Bi < 0.1, and effectively that means particles of about 600 μm.

The biomass volatile yields used were based on the measured laboratory value of VM and a correction obtained from using the FG-Biomass program.

Table 3. Volatile Yields for the Biomass Fuels

Biomass	VM (daf)	Calculated by FG-Biomass	Value given by RWE npower
Milled wood	86.58.7	90.91	76.34
PKE	93.13	97.79	85.54
Olive	75.71	79.50	
Miscanthus	80.8	84.8	
Torrefied wood	75	80	

2.3 Water Evaporation Model

The moisture level in solid fuel can play a significant role in the combustion process. In coal it is usually about 3% but in industrial coals stored in the open it may reach 10%. Freshly harvested biomass contains a significant amount of water, often up to 50% although once air-dried, as in this project, it is still about 5-10 %. The evaporation of water from biomass presents a number of problems because of the non-homogeneous nature of the samples. Moisture release is therefore difficult to predict and consists of two parts-evaporation of liquid water and the evaporation of water in capillaries.

Many drying models have been developed and all computer models contain an expression to allow for this. It is assumed that the progress of drying is limited by the transport of heat inside the particle and the moisture evaporation rate is effectively that of an evaporating droplet. The major assumption is that the particle is assumed to have a uniform temperature profile across it (as determined by the Biot Number)
Many materials are anisotropic and the evaporated water has an effect on particle motion and causes rotation and jet effects but this was not taken into account.
In this way the heating-up curves for the influence of moisture on ignition delay can be calculated as shown in Figures 4a-c.

At the burner exit and prior to combustion the velocity of the particles is about 5-9 m/s, so a particle travels say 5-9 mm/ms. If the curves calculated in Figure 4a hold then the ignition of a 0.5mm diameter particle would be delayed by 10 ms, that is 0.5 cm., Of course larger particles, say 1mm in diameter and containing significant amounts of water would penetrate further, possibly several cm as indicated by Figure 4c or larger ultimately resulting in incomplete burnout.

Figure 4 (a) Heating-up Curves for Biomass Particles (0.5 and 1mm diameter 5%water content)
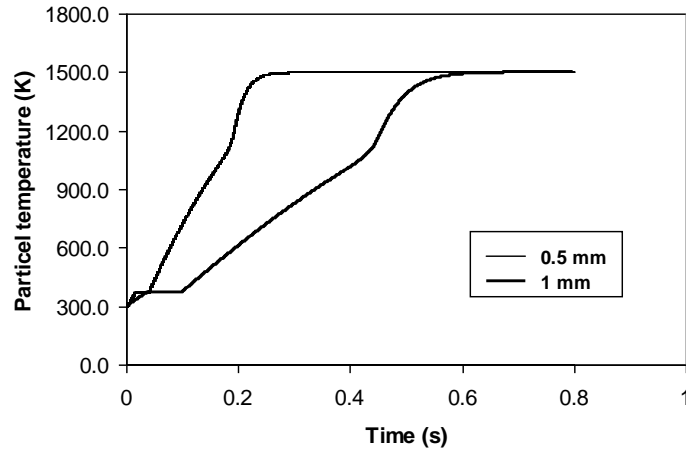

Figure 4 (b) Time to Ignition (taken as the end of water evaporation) as a function of moisture content for different sized particles and temperature
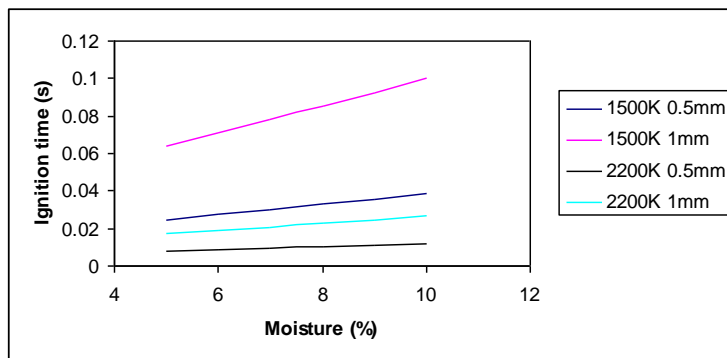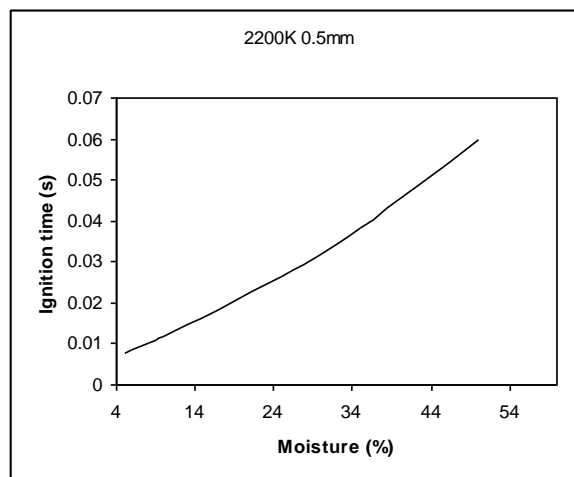

Figure 4 (c) Plot of Ignition Times for high moisture levels, 0.5 mm and 2200K

2.4 NOx and Soot Models

These have been described in previous publications [4] and are effectively the Fluent default models with some adjustment to the approach used. In the case of coal the fuel-N is converted to HCN with the subsequent calculation estimating the amount of NO and N_2 produced depending on the stoichiometry. With biomass the situation is more complex because both HCN and NH_3 are formed from the protein and amino acids which contain the nitrogen [7]. Within Fluent there are reaction routes via either NO or NH_3 and not both and the way this is handled here is discussed in Section 3. For the soot model, we used the mechanism outlined by us in reference [4]. But the issue is the amount of soot formed-there is an adjustable constant-this was done in the analysis below.

The Fluent overall single-step soot prediction model was used based on the total volatile concentration. The rate of soot formation is given by an empirical equation below and the combustion of the soot particles was governed by the Magnussen equation.

$$\mathcal{R}_{\text{soot,form}} = C_s p_{\text{fuel}} \phi^r e^{-E/RT}$$

The choice of the soot formation constant, C_s, and the activation energy, E_s, for a number of fuels has been discussed [4, 17]. Previously we chose constants for the volatiles in these bituminous coals on the basis of their C/H ratio (approximately 1.5) as: equivalence ratio exponent, r, is equal to 3; the activation temperature E_s/R is 2000 K; soot formation constant, C_s, is 1.5. The stoichiometric coefficient for soot combustion was taken to be 2.7 and the Magnussen constant for soot combustion as 4. The model was computed with soot-radiation interaction. In this study the value of Cs was varied as discussed later in Section 3b.

2.5. Validation of the CFD model in the RWE npower Combustion Test Furnace: Combustion of a single Coal, Gascoigne Wood.

There is a considerable amount of experimental data available for the combustion of Gascoigne Wood and consequently this data was used to test some aspects of the CFD model. There are a number of issues:

(a) **Turbulence Models.** Some studies were undertaken with different turbulence models for the combustion of Gascoigne Wood coal. The experimental furnace exit temperature is 1597 K and the results for the different turbulence models are given below
ED-RNG – eddy dissipation model with RNG turbulence model-   1700 K
ED-SKE -- eddy dissipation model with standard k-epsilon turbulence mode-1650 K
PDF-SKE – pdf model with standard k-epsilon turbulence model-   1420 K

It seems that the best agreement in terms of the exit temperature and the position of the maximum of the radiation flux is obtained with the ED SKE model. In order to test the sensitivity of the model to the heat input parameter the heat of combustion was increased by 15%. The computed temperature in this case was 1580 K. Thus about 1% error in the heat of combustion leads to a 10$^{\text{o}}$C change in temperature.

Since there can be variations in the composition and the firing rate of approximately 5%, fluctuations in the order of 50 °C can readily occur. The choice of the turbulence model and the devolatilisation model also determines the flame stability (flame holding) and the flame shape. The general view of the flame in the furnace is shown in Figure 5a and the detailed near-burner structure in Figure 5 b.

Figure 5 (a). General View of the Contours of Static Temperature (Gascoigne Wood Coal Combustion)
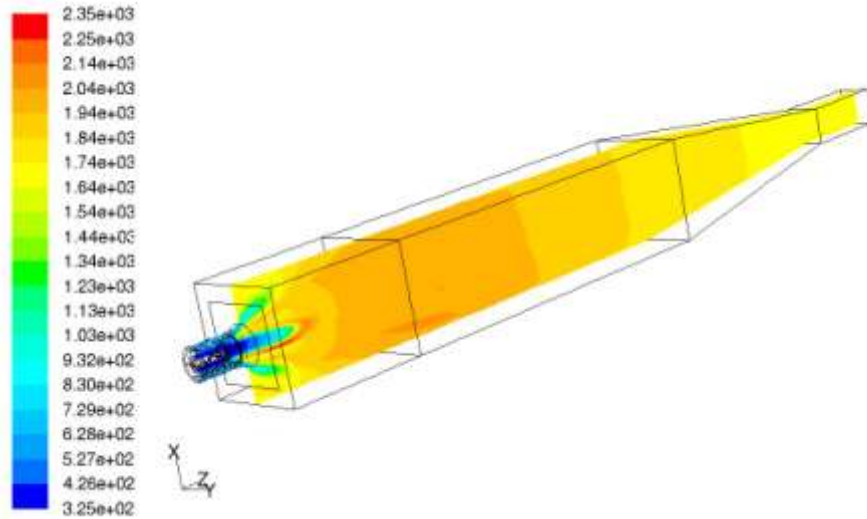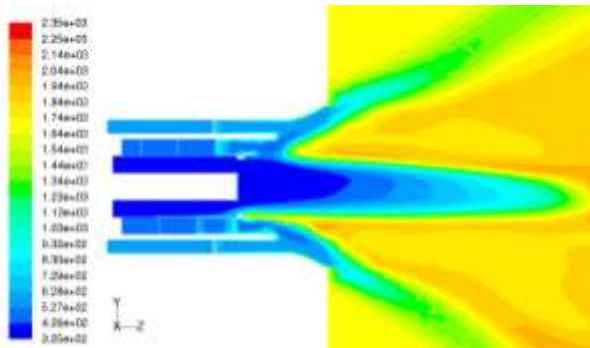

Figure 5 (b). Flame Attachment Detail (for Gascoigne Wood Coal Combustion)

A photograph of this flame provided by RWE npower is shown below.

Figure 5 (c), Photograph of the Flame

There is reasonable agreement on the position of flame attachment, ignition, and flame shape. This was determined using a densitometer to obtain a quantitative measurement of the flame shape and intensity as a function of the distance from the flame. The expansion angles are the same as is the general flame shape.

(b) Investigation of the Radiation Properties of the Flame.

There was experimental data available from RWE npower for this flame on the incident flux to the furnace wall, and there was information available from related investigations [17, 18] on flame temperatures measurements. This information was compared with our computed data.

The first issue is the choice of radiation model and for this investigation we used the DO model whereas previously we used the P1 model. This was done because this is a more detailed and accurate model but more demanding on computational time. However more powerful computers are available and this is now our first choice.

As far as the temperatures there is reasonably good agreement with measured temperatures (for a similar coal, not Gascoigne Wood)) as shown below.

Figure 6. Measured Temperature Field [18, reproduced with permission]: red, 1650°C; yellow,1580°C; blue/green, 1450°C.
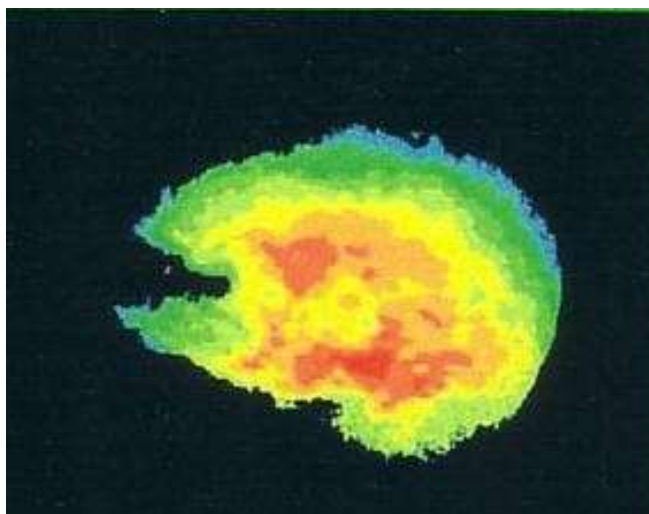
Information was provided by RWE npower on the radiant fluxes in the furnace obtained using a Medtherm heat flux transducer (H 201, optical range 0.15-5 μm, accuracy +/- 3%). These results are shown in Figure 7 below together with the computed values.

It was not possible to obtain a very close match as shown in Figure 7 below There are a number of factors that can come into play and these are

    (a) the accuracy of the emissivity data. We note that in recent published work [20] different values were used to the ones commonly accepted and used by us.

    (b) The accuracy of the model particularly in circumstances where there are some simplifications to the furnace geometry

    (c) The accuracy of the measurements-and particularly the degree of coincidence of the measured case and the computed one.

Figure 7. Surface Incident Radiation Measurements and Computation (Gascoigne Wood): Heat flux as a Function of Distance (m)
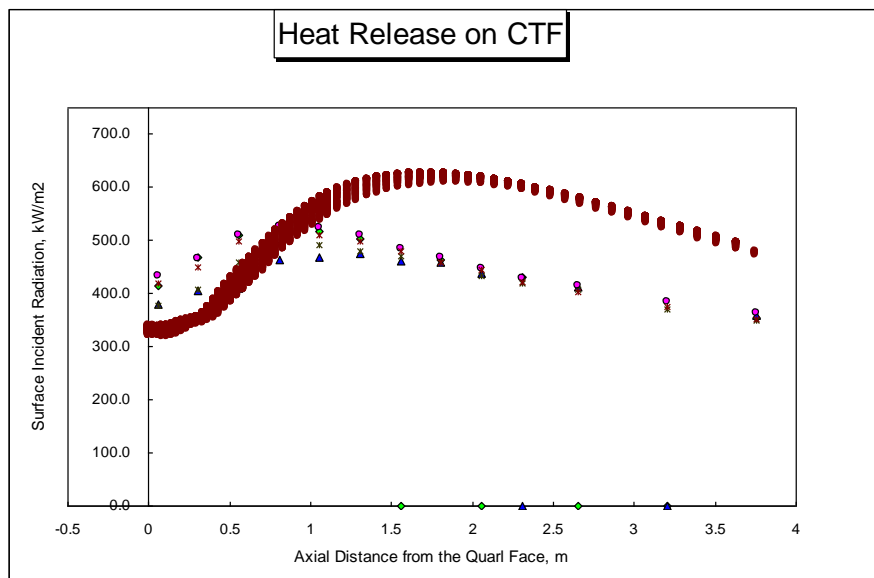
The radiative contribution of the soot was tested by varying the soot formation parameter. About the soot calculation, on increasing the 'Soot Formation Constant' from the default value 1.5 (kg/N-m-s) to 7.5, the highest incident radiation increased by about 10%, and the location moved slightly towards the burner. However the shape and the maximum value of the radiation flux are not absolutely correct which could rise from (a) incorrect value being used for the devolatilisation, (b) incorrect chemical reaction mechanism which does not include the option of free radicals in the recirculated gas stream igniting the fuel, and (c) incorrect measurement of the radiant flux near the burner; there is some evidence that similar effects have been observed in furnace measurements in other research institutions possibly due to the complex

geometry where the burner enters the furnace. These calculations are being considered further because recent measurements of coal particle emissivity indicate that there is a significant change as the particle moves from the flame front to the main part of the combustor [30].

3. Co-Combustion of Coal and Biomass in the Combustion Test Facility.

On the basis of the studies with the Gascoigne Wood coal the model was used for the co-firing studies, but there are additional factors in the case of biomass relating to the nature of the biomass particles.

(a) The Heating-up Equations. The equations used are those described in the Fluent manual where there are problems due to the choice of Cp and the fact that the biomass has a different emissivity to coal.

(b) The Aerodynamic Equations

The equations used are the standard Fluent equations but the large biomass particle sizes present a problem. The drag coefficients, C_D, are as in equation (1) and shape factors were used to account for the irregular biomass particles shapes.

$$C_D = (24/Re)(1 + b_1 Re^{b_2}) + [b_3 Re/(b_4 + Re)] \qquad (1)$$

$$b_1 = 2.3288 - 6.4581f + 2.4486f^2 \qquad (2)$$

$$b_2 = 0.0964 + 0.5565f \qquad (3)$$

$$b_3 = 4.9050 - 13.8944f + 18.4222f^2 - 10.2599f^3 \qquad (4)$$

$$b_4 = 1.4681 + 12.258f - 20.7322f^2 + 15.8855f^3 \qquad (5)$$

b_1, b_2, b_3 and b_4 are expressed in terms of the shape factor, f, which is defined as the ratio of the surface area of an equivalent sphere having the same volume as the particle and the actual surface area of the particle.

As far as the combustion of the large particles they seem to generally follow the same laws as coal particles. Examination using video images showed that suspended particles had the expected ratio of the radius of the flame zone/radius of the particle. Examination of this radius ratio provides confirmation of the amount of volatiles associated with the devolatilisation of the biomass particles. Likewise examination of the video gives confirmation of the burning times. Some jetting of material took place at the ends of the particles which could cause tumbling in a flame but the effect was considered not to be a major factor and not included in the calculations.

Figure 7. Examination of the Combustion of a Single Particle of Wood

In these flames it is possible to quantify the ratio $_{of}$ the flame zone radius to the particle radius (r_c/r_p) and make conclusions about the rate of evolution of the volatiles and indeed the NO and smoke release. This will be followed up in a future project under SuperGen-Bioenergy.

(c) Flame Shapes.

Comparisons could be made of the computed flame shapes with experimental studies. A typical flame is shown below and it has a well-defined flame shape with the flame edge diverging from the centerline at an angle of 10°. In principle it is possible to quantify these flame parameters but there has not been an opportunity to do this to any extent in this project.

Figure 8. Experimental Furnace Flame Shape

Generally biomass flames are attached more firmly to the burner and have a larger flame divergence angle, both consistent with the higher reactivity of the biomass and the larger quantity of volatiles produced.

(d) NOx Calculations for Biomass.

Generally woods contain about 70-90% protein an amino acids and this is a reasonable assumption for miscanthus too. In the case of PKE, Olive waste and torrefied wood the same assumption is made. In that case we have followed the

method previously used by us [7] and assumed that the ratio of NO produced via HCN and NH$_3$ routes is 1:3. Effectively in the case of a 20% biofuel the actual NOx is 10% higher than if this route is not taken into account.

Computations were carried on the basis described and the results are given in the Table below.

Generally the computed results are in reasonable agreement with the experimental results. There are a number of factors that influence the accuracy of the experimental results. These include the experimental errors for the individual measurements (typically 5% although the C-in-ash values are more like 20%), but a major factor is that the experiments are made under conditions where the furnace is being used to undertake a large number of commercial data collection operations and is not operating under steady state temperature conditions. Therefore the input data for the CFD calculation does not exactly match the conditions under which the experiment data were obtained.

Table 4. Comparison of Experimental and Computed Data.

Fuel	Calc NO ppm (dry)	Measured NO ppm (dry)	Calc C in Ash, Mass %	Measured C in Ash, Mass %	Calculated exit T, K	Experimental Exit T, K
Gascoigne Wood coal	313	325	1.32	3.0	1605	1597
Russian coal	296	325	1.24	3.4	1617	1407
Russian/PKE	316	321	3.5	4.8	1487	1488
S. African coal	330	312	5.87	6.7	1668	1424
S. African coal/ wood	288	319	5.6	5.9	1583	1527
S. African/ Miscanthus (20%)	236	242	8.9	1.94	1664	1470
S. African/ Olive waste (15%)	276	230	0.62	0.98	1646	1539
S. African/Torrefied Wood* (20% thermal)	239	Not available	0.3	Not available	1724	Not available

*Assuming the milled wood has a particle size which is the same as coal.

4. Discussion and Conclusions

The Combustion Test Facility has been modelled using a single coal. In the validation studies with Gascoigne Wood coal reasonable agreement with the experimental results were obtained although there is still some uncertainty about the radiation data.

The coal and biomass models give a satisfactory prediction of the combustion properties. In particular we have the major char combustion and a devolatilisation

model that includes prediction of the rates and yields and no experimental measurements are necessary. It has been possible to deal with complex particle particle sizes and shapes in a reasonable manner. Attention has been drawn to the importance of accurate data on the specific heats of the coals and in particular of the biomass particles.

The computer model has been modified to improve the accuracy of the temperature predictions and it has been run using three coals and four coal/biomass mixtures, and a hypothetical case of a blend containing torrefied wood. The latter case was studied because of the current interest in the combustion of this pre-processed fuel. The agreement between computed and experimental radiation results is not precise and this could arise from a number of issues ranging from the conclusions about the kinetic rate through to the turbulent model used. It is our intention to revisit the issue of radiation modelling in a future project.

Computations undertaken using the N-model to compute the NOx were satisfactory as were the calculations of the unburned carbon-in-ash, although greater sophistication is required and this is being addressed by current research under the SuperGen-Bioenergy project.

The major issues that caused problems are the fact that the research facility was designed for industrial testing rather than for an academic study, and therefore lacked extensive combustion diagnostic equipment of the type required for a detailed academic study. It would be an extremely advantageous to run such a rig using the instrumentation that is available to UK research institutions via the EPSRC Equipment Loan Bank using a systematic range of highly characterised coals and biomass fuels.

The Project has provided information of value to groups using CFD modelling of coal and coal-biomass blends for furnace prediction for industrial power station design purposes.

5. Acknowledgements

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List of Publications
1. L. Ma, M. Pourkashanian, J.M. Jones and A. Williams A. Co-firing Pulverised Coal with Biomass in Industrial Furnaces, 6th European Conference on Coal Research and its Applications, University of Kent, Canterbury, Kent 5th – 7th September 2006
2. L. Ma, M. Pourkashanian, J.M. Jones and A. Williams A The Effect of Moisture Content on the Ignition of Biomass Particles, To be published, Journal of the Energy Institute, 2008
3. L. Ma, M. Gharebaghi, R. Porter, M. Pourkashanian, J M Jones and A. Williams, Modelling Methods For Co-Fired Pulverised Fuel Furnaces, Paper submitted to the 7th European Conference on Coal Research and its applications, Cardiff University, 2008
4. Y.B. Yang, V.N. Sharifi and J. Swithenbank, L. Ma, L.I. Darvell, J.M. Jones, M. Pourkashanian and A. Williams, Combustion of a Single Particle of Biomass, Energy and Fuels, 22, 306-316, 2008.

Appendix 1   Details of the Burner and Furnace

Details of the 0.5 MW Doosan Babcock Mark III burner are shown below.

A 1.1. Burner Face Details
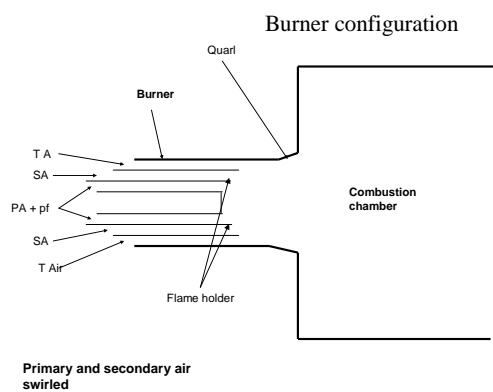

The inside of the furnace is shown below indicating the positions of the ports used for the radiation measurements.

A 1.2. Furnace Geometry

A 1.3. Diagrammatic Representation of the Doosan Babcock Mark III Burner

Appendix 2. Details of the Char Model

The models have been described in earlier publications particularly the devolatilisation model based on FG-DVC [2]and the char model [4], and these also give details of the nomenclature used. The char model used here includes a number of extra features and these are indicated below.
The conventional char combustion model is:

$$(dm_p/dt) = \pi \, d_p^2 \, [(\rho_p \, R \, T_\infty \, Y_{ox})/M_{w, \, ox}] \, [D_0 \, \Re/(D_0+\Re)] \qquad (6)$$

where

t	time
d_p	char particle diameter
ρ_p	char particle density
T_∞	environment gas temperature
Y_{ox}	local mass fraction of oxidant species in gas surrounding combusting char particle
$M_{w, \, ox}$	molecular weight of oxidant species in gas surrounding combusting particle
D_0	diffusion rate coefficient
$\Re$	kinetic rate incorporating effects of chemical reaction on internal surface of char particle (intrinsic reaction) and pore diffusion

1. Non-default values were selected foe intrinsic char model parameters [4]: mass diffusion limited rate constant, kinetics limited rate pre-exponential factor and mean pore radius, to improve/optimise the accuracy of the calculated char combustion rate

2. Inclusion of a variable char particle surface area scaling factor, f_{scal} (7) (8) within the intrinsic char burning rate expression (6), via user-subroutines, where $A_{p, \, i}$ represents the specific internal surface area of the char particle and k_i represents the intrinsic char particle reactivity. =

$$\Re = A_{p, \, i} \, \eta \, (d_p/6) \, \rho_p \, k_i \qquad (7)$$

$$\alpha = f_{scal} \, (-28.44 \, B_C^4 + 85.33 \, B_C^3 - 85.33 \, B_C^2 + 28.44 \, B_C + 1) \qquad (8)$$

3. Inclusion of a coal maceral correction factor, f_{mac}, as described previously [4], within the char burning rate expression (5), via user-subroutines. Thus the char burning is determined by the maceral composition.

4. Inclusion of a simplified thermal annealing correction factor, f_{ann} (9), within the char burning rate expression (5), via user-subroutines, where C_p represents the carbon content of the char particle.

$$f_{ann} = 0.9 \text{ if } \{70 \, \%wt < C_p < 90 \, \%wt, \, 20 \, \mu m < d_p < 100 \, \mu m, \, T_p > 1400^o C\} \qquad (9)$$

5. Thus we have simulation of of char combustion for different coals where $\Re$ is represented by (7) and (8).

$$(dm_p/dt) = f_{ann} \, f_{scal} \, \pi \, d_p^2 \, [(\rho_p \, R \, T_\infty \, Y_{ox})/M_{w, \, ox}] \, [D_0 \, \Re/(D_0+\Re)] \qquad (9)$$

Appendix 3 Coal and Biomass Properties

Table A 3.1. Coal Properties (%as received)

Coal	Gascoigne Wood	Russian	South African
Inherent moisture	4.00	5.56	5.47
Ash	17.74	12.15	12.15
VM	27.48	36.19	30.01
FC	50.78		
C	63.99	65.42	67.01
H	4.21		
N	1.36	1.54	1.56
S	1.112	0.44	0.48
Cl	0.05		
GCV MJ/kg	26.47	26.83	26.75
GCV MJ/kg	25.44		

Table A 3.2. Biomass Properties (%as received)

Biomass	PKE	Olive waste	Milled wood	Miscanthus	Torrefied wood*
moisture	9.22	6.41	7.79	8.42	1.0
ash	3.9	7.96	2.4	5.45	8
VM	80.26	64.83	77.76	69.57	71
FC	6.62	20.8	12.05	16.56	20
C	44.91	46.42	47.51	42.81	
H		5.70	5.92	5.34	
N	2.43	1.08	0.32	0.50	0.7
S	0.22	0.13	0.005	0.08	
Cl					
K			0.4		
GCV MJ/kg	18.72	18.60	18.61	24.93	21.8
NCV MJ/kg					

*Torrefaction temperature-563 K

Appendix 4. Summary of Kinetic Analysis

The plot below shows the variety of data available for kinetic studies. The central black area shows data from wire mesh (mainly for coal) and from TGA studies (both for coal and for biomass). Higher rates are obtained from drop tubes and open laboratory flames but without surrounding radiating walls. The highest rates are applicable to high intensity flames in radiant furnaces and these are used here based on the assumption that these simulate real furnace flames..

Figure A 4. Plot of Rate Constants as a Function of temperature