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# CFD MODELING OF THE OXY-FUEL COMBUSTION OF VICTORIAN BROWN COAL IN DROP TUBE FURNACE AND 3MW PILOT SCALE BOILER

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## ABSTRACT

With Victorian brown coal being responsible for electricity generation in the state, minimising the environmental impact of its combustion is vital for the sustainable use. Oxy-fuel technology is one promising and cost-effective option for carbon capture and sequestration in both short and medium terms. Due to the presence of abundant moisture within it, *i.e.* up to 70 wt%, Victorian brown coal combustion possesses numerous distinct characteristics in oxy-fuel combustion. In this study, a series of CFD modelling has been conducted by using Ansys-Fluent to clarify pulverized coal flame ignition and propagation in oxy-fuel process, and its variation with coal moisture content. First, the simulation focused on particle temperatures under different oxy-fuel conditions in a lab-scale drop tube furnace (DTF). The pulverized coal particle temperature in 27 vol% $O_2$ balanced by $CO_2$ was found agreeing with conventional air-combustion mode. Such a phenomenon was further confirmed by simulating coal combustion in a 3 MW pilot boiler. Moreover, modelling a wet coal containing 30% moisture indicated the expansion of pulverized-coal flame length and char ignition delay.

## NOMENCLATURE

| | |
|---|---|
| $A_p$ | Particle external surface area |
| $d_p$ | Particle size |
| $f$ | Mixture fraction |
| $g$ | Acceleration of gravity |
| $H_{reac}$ | Reaction heat of $C+O_2=CO_2$. |
| $k$ | Turbulent kinetic energy |
| $m_p$ | Particle mass |
| $P_{O2}$ | Oxygen partial pressure at ambient |
| $T_\infty$ | Ambient temperature, |
| $T_p$ | Particle temperature. |
| $u_i$ | Gas-phase velocity |
| $u_{pi}$ | Particle velocity |
| $\rho_p$ | Particle density |
| $\sigma$ | Stefan-Boltzmann constant |
| $\alpha$ | absorption coefficient, |
| $\sigma_s$ | scattering coefficient |
| $\Omega$ | solid angle |
| $\varepsilon_p$ | particle emissivity |
| $\varepsilon$ | turbulent kinetic energy dissipation rate |

## INTRODUCTION

Victorian brown coal is the single largest source contributing to the electricity needs in Victoria. However, its combustion is also the major contributor for greenhouse. In particular, the abundant moisture in Victorian brown coal, up to 70 *wt%*, is the major cause increasing its carbon emission rate per electricity output. There are several ways for carbon capture and storage (CCS), such as pre-combustion capture by gasification, post-combustion, and *in situ* via oxy-fuel combustion technology. Of those, oxy-fuel combustion is considered the most promising and cost-effective, as it requires minimal infrastructure modification for the retrofit of existing plants or construction of a purpose-designed boiler. During oxy-fuel combustion, the conventional air is replaced by the mixture of high-purity oxygen ($O_2$) and recycled flue gas (RFG), which generate a $CO_2$-rich flue gas that is potentially subjected to direct sequestration.

In the work, a series of modellings have been conducted to validate the experimental observations for the oxy-fuel combustion of Victorian brown coal, either dry or wet, in a lab-scale drop tube furnace and a 3MW pilot scale boiler.

## MODEL DESCRIPTION

Pulverized coal combustion is a very complicated physical and chemical process, which is related to gaseous turbulent flow, two-phase flow involving solid particles, homogenous gaseous reactions, heterogeneous surface reactions, radiation heat-transfer, *etc*. Generally, the amount of unburnt carbon depends on particle residence time in furnace, gas temperature and the availability of oxygen along particle path. Therefore, an accurate prediction of coal combustion rate is essential to assess particle temperature and heat transfer profile. In this article, a commercial CFD software, Ansys-FLUENT-13.0 has been used. The sub-models used are summarised as follows.

### (1) Realizable k-ε model for gaseous turbulence model

The k-ε model is the most popular turbulent model based on the Reynolds time-averaged Navier-Stokes (RANS) equations. Realizable *k-ε* Model, an improved *k-ε* Model, is able to predict the strong swirling flow, and hence it is applicable for the numerical simulation in a tangentially-fired furnace.

**(2) Particle random trajectory model for particle motion calculation**

There are two different approaches to treat the gas-particle two-phase flow: one is to consider gas as a continuum and particles as a discrete system, namely particle trajectory model, and the other is to consider both gas and particles as co-existing and interpenetrating continua or particles as a pseudo-fluid, namely multi-fluid model. The feasibility of these two models depends on particle volume fraction, relaxation time and particle-particle impact time. The particle random trajectory model was employed here, which is a coupling of gaseous turbulence on the Eulerian coordinate with the particle motion on the Lagrangian coordinate. It's assumed that coal particle has a spherical shape and its particle diameter obeys the Rosin-Rammler distribution. During combustion, coal particle size is assumed to remain constant, while the particle density varies. The particle motion is described in Equation 1.

$$\frac{du_{pi}}{dt} = F_D(u_i - u_{pi}) + \frac{g_i}{\rho_p}(\rho_p - \rho) \quad (1)$$

where $F_D = \frac{C_D \operatorname{Re}_p}{24\tau_r}$, $\tau_r = \frac{d_p^2 \rho_p}{18\mu}$, $\operatorname{Re}_p = \frac{\rho d_p |\vec{u} - \vec{u}_p|}{\mu}$

$$C_D = \frac{24}{\operatorname{Re}_p}(1 + b_1 \operatorname{Re}_p{}^{b_2}) + \frac{b_3 \operatorname{Re}_p}{b_4 + \operatorname{Re}_p}$$

With regard to the influence of random turbulence on particle motion, the gas fluctuation velocity ($u_i'$), obeying a stochastic distribution of Gaussian PDF, is used to calculate real particle trajectories.

$$u_i' = \zeta(\overline{u_i'^2})^{1/2} = \zeta\left(\frac{2k}{3}\right)^{1/2} \quad (2)$$

Where $\zeta$ is random number with Gaussian distribution.

**(3) Non-mixed combustion model for the turbulent gas reactions in the coal air-combustion case**

The non-mixed combustion model, viz. simplified PDF fast-reaction model, assumes that kinetic reaction rates of gaseous fuel are sufficiently fast and the overall combustion rate is controlled by gas diffusion. In the non-premixed combustion model, char and volatile are considered as two independent fuels flow while air is treated as the oxidizer. The influence of turbulence is considered by the probability density function (PDF) where a $\beta$ function is used in FLUENT.

Time -average equation of mixture fraction:

$$\frac{\partial}{\partial t}(\rho\bar{f}) + \nabla\cdot(\rho\vec{v}\bar{f}) = \nabla\cdot\left(\frac{\mu_t}{\sigma_t}\nabla\bar{f}\right) + S_m \quad (3)$$

Mixture fraction variance equation:

$$\frac{\partial}{\partial t}\left(\rho\overline{f'^2}\right) + \nabla\cdot\left(\rho\bar{v}\,\overline{f'^2}\right) = \nabla\cdot\left(\frac{\mu_t}{\sigma_t}\nabla\overline{f'^2}\right) + C_g\mu_t\left(\nabla^2\overline{f}\right) - C_d\rho\frac{\varepsilon}{k}\overline{f'^2} \quad (4)$$

This model is often used to predict the simulation in coal-air combustion. However, it is not applicable to oxy-fuel combustion because of its limitation of setting boundary conditions, *i.e.* inlet species concentration, by using mixing fraction.

**(4) Finite-rate/eddy-dissipation model in the coal oxy-fuel combustion case for turbulent gas reactions**

Finite-rate/eddy-dissipation model considers two control mechanisms, Arrhenius laminar reaction mechanism and turbulent fluctuation mechanism. The eddy dissipation model (EDM) was developed from the eddy break-up (EBU) model, firstly proposed by Spalding.

**(5) Discrete-ordinate (DO) radiation model**

In the power plant furnace, the fraction of radiative heat-transfer could achieve as high as approximately 95%. The radiative transfer equation using DO model is written as

$$\nabla\cdot\left(I\left(\vec{r},\vec{s}\right)\vec{s}\right) + (a + \sigma_s)I\left(\vec{r},\vec{s}\right) = an^2 I_{b\lambda} + \frac{\sigma_s}{4\pi}\int_0^{4\pi} I\left(\vec{r},\vec{s}\right)\Phi\left(\vec{s},\vec{s}'\right)d\Omega' \quad (5)$$

Considering the affect of green gases ($CO_2$ and $H_2O$), the weighted-sum-of-gray-gases model (WSGGM) is used for computation of a variable absorption coefficient, which helps improve the accuracy of radiative heat transfer in an oxy-fuel furnace.

**(6) Pulverized coal combustion model**

The combustion of pulverized coal can be divided into different processes, including preheating, devolatilization, volatile release/combustion and char combustion.

The kinetics/diffusion control model is used for char combustion. In this article, only C-$O_2$ reaction is considered, the rate of which is expressed as:

$$\frac{dm_p}{dt} = -\pi d_p^2 P_{O2}\frac{k_d k_s}{k_d + k_s} \quad (6)$$

Diffusion limited coefficient $k_d = C_1\frac{\left[(T_p + T_\infty)/2\right]^{0.75}}{d_p}$

Where $C_1$ is equal to $5\times10^{-12}$ and $4\times10^{-12}$ for air combustion and oxy-fuel combustion, respectively, .

Kinetic limited coefficient $k_s = C_2\exp(-E/RT_p)$

The energy conservation of a coal particle can be expressed as the balance of particle internal energy and convective/radiative heat transfer:

$$m_p c_p\frac{dT_p}{dt} = hA_p(T_\infty - T_p) + A_p\varepsilon_p(\theta_R^4 - \sigma T_p^4) + f_h\frac{dm_p}{dt}H_{reac} \quad (7)$$

Where $f_h$ is energy distribution coefficient (=0.3), assuming that only C + $0.5O_2$=CO occurs at particle surface and CO oxidation has a freezing state in particle boundary layer.

## MODELING 1 FOR OXYFUEL COMBUSTION IN DROP TUBE FURNACE

A lab-scale DTF used for coal combustion is illustrated in Figure 1 for its schematics. It is useful to provide a one-dimensional gas flow and sufficient information to understand the fundamentals of coal combustion in different gases. The furnace is 2.0 m long and consists of six heating sections that are controlled individually. A 3D model of the DTF was drawn using software ANSYS-Gambit, as shown in Figure 2. The total structural mesh number is 125,600.

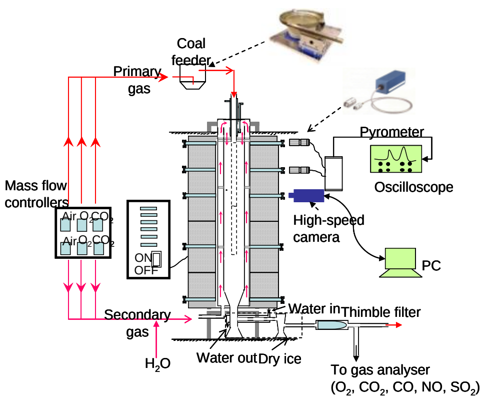



**Figure 1:** Schematic drawing of the DTF

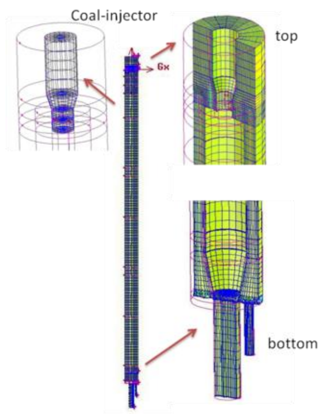
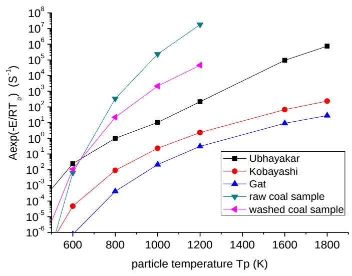



**Figure 2:** Modelling geometry of DTF

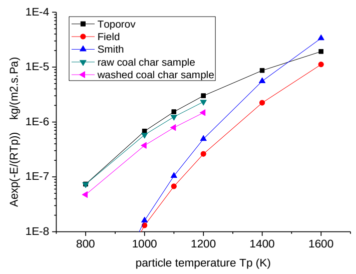
**Table 1:** Properties and Kinetic reaction rate of Victorian brown coal obtained by TGA

| | | | | |
|---|---|---|---|---|
| (1) Proximate analysis, %db | | | | |
| Moisture, %ar | Ash | | Volatile matter | Fixed carbon |
| 10.1 | 3.0 | | 50.1 | 46.9 |
| (2) Ultimate analysis, %db | | | | |
| C | H | | N | S |
| 67.1 | 4.9 | | 0.6 | 0.5 |
| (3) Volatile release rate | | | | |
| | | Pre-factor ($s^{-1}$) | Activation Energy (KJ/mol) | |
| raw coal | | $5.18\times10^{16}$ | 217.27 | |
| Washed coal | | $1.92\times10^{11}$ | 152.22 | |
| (4) Char oxidation rate | | | | |
| | | Pre-factor ($kg/(m^2s)$) | Activation Energy (KJ/mol) | |
| raw coal | | 0.0024 | 69.06 | |
| Washed coal | | 0.0014 | 68.54 | |

The kinetic data of Victorian brown coal was measured by Thermal gravity analysis (TGA) in this study, which was used in modelling. The comparison between Victorian brown coal and other coals in literature was shown in Table 1 and Figure 3. As can be seen, the air-dried Victorian brown coal possesses higher reactivity for devolatilisation and char oxidation reactions than referred black coals. Moreover, the Victorian raw coal sample has better reactivity than washed coal sample.




(a)Volatile release rate




(b) Char oxidation rate

**Figure 3:** Kinetic reaction rate obtained by TGA and comparison with some kinetics reported in literatures

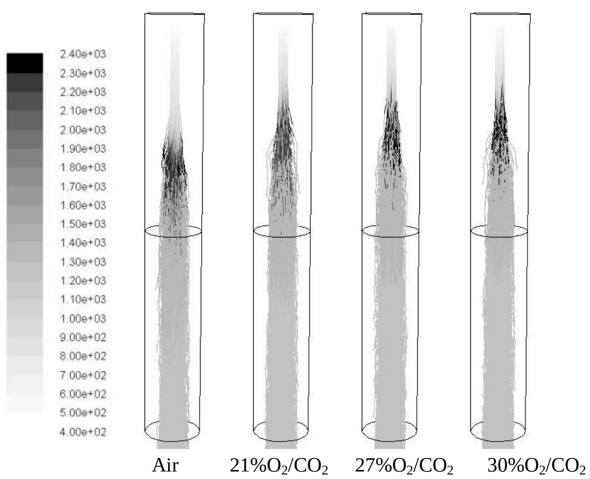



**Figure 4:** Predicated particle temperature profile in DTF under gas conditions of air, 21%$O_2$/$CO_2$, 27%$O_2$/$CO_2$ and 30%$O_2$/$CO_2$

For each run in drop tube furnace, coal was entrained by 1.0 L/min primary gas and fed at a rate of about 0.5 g/min. Secondary gas was introduced at a flow rate of 9.0 L/min from the bottom of the outer chamber of the reactor, which was heated up to the furnace temperature 1000℃ before entering combustion zone. The predicted particle temperatures are shown in Figure 4. As can be seen, using the same amount of oxygen in $CO_2$ as in air, *i.e.* 21%, creates the lowest temperature for burning coal particles. This is due to the larger specific heat capacity of $CO_2$ than $N_2$, which significantly retards coal ignition and flame combustion. Increasing the oxygen content to 27% is good enough to offset the negative effect of $CO_2$, leading to a similar temperature profile for burning coal particles in the furnace.

## MODELING FOR OXYFUEL COMBUSTION IN A PILOT-SCAL 3MW BOILER

The 3.0 MW pilot scale boiler was designed as the Π-type structure. The boiler geometry is shown in Figure 5. The cross sectional size of the furnace is 1200mm×1200mm. The flue zone has slightly smaller cross sectional area, which is 1200mm×800mm.

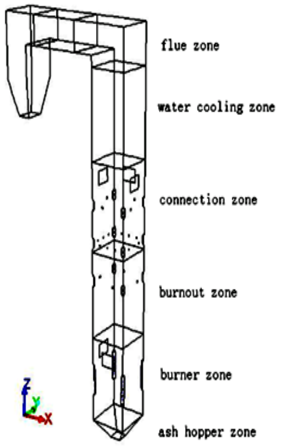



**Figure 5:** Schematic drawing of 3MW boiler

The drawn geometry was discretized into a collection of meshes. Considering that the accuracy of the calculation highly depends on the quality of meshes, the meshes in the cross sections of burner zone and OFA zone were drawn in Figure 6. Approximately 143,000 meshes were created. In each primary air inlet, 45 dots were defined as the particle phase starting points. And in each coupling calculation, 3,600 particles trajectories were tracked respectively.

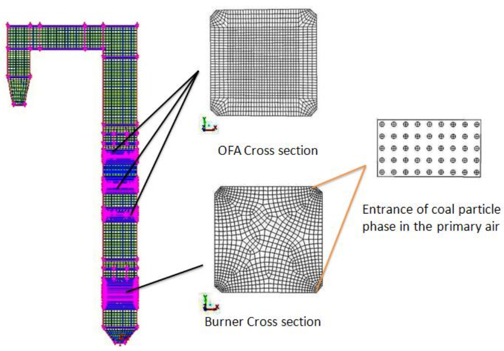



**Figure 6:** Modelling geometry of 3MW boiler

The experiment of burning a Chinese mixed coal in air was first conducted to help establish and validate the numerical models employed in this study. The coal properties and operation conditions are tabulated in Tables 2 and 3. The gas temperature profile calculated by CFD is demonstrated in Figure 7, which shows a good agreement with the experimental observation (symbols in figure 7) and validates the models. Moreover, the predictions by non-mixed combustion model are very close to the results from using the finite-rate/eddy-dissipation model for air combustion mode.

**Table 2:** Coal properties used in 3MW boiler

| | A Chinese mixed coal | Victorian brown coal |
|---|---|---|
| (1) Proximate analysis ( wt% db) | | |
| Moisture (ar) | 11.53 | 16.6 |
| Ash | 9.32 | 0.7 |
| Volatile matter | 32.82 | 49.9 |
| Fixed carbon | 52.11 | 49.4 |
| (2) Ultimate analysis (wt% db) | | |
| C | 69.54 | 70.2 |
| H | 6.24 | 4.7 |
| N | 0.69 | 0.52 |
| S | 0.46 | 0.35 |
| (3) High heating value as received | | |
| HCV KJ/Kg | 28.424 | 22.75 |

**Table 3:** air combustion experiment cases burning a Chinese mixed coal in 3MW boiler

| | Modeling | Experiments | | |
|---|---|---|---|---|
| Thermal power (MW) | 1.9 | 1.889 | 1.897 | 2.013 |
| Total coal flux (kg/h) | 271.9 | 270.3 | 271.53 | 288.14 |
| Excess air coefficient | 1.27 | 1.27 | 1.28 | 1.25 |
| Total primary air ($Nm^3/h$) | 400.0 | 372.8 | 383.1 | 376.84 |
| Total secondary air ($Nm^3/h$) | 2051.2 | 2044.7 | 2045.4 | 2179.86 |

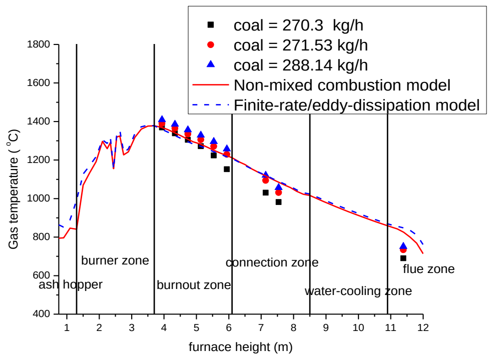
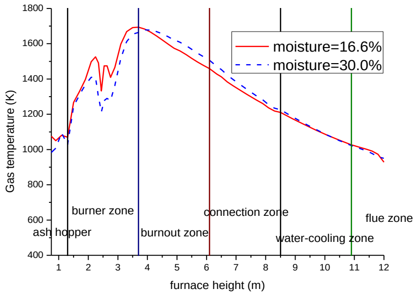



**Figure 7:** Comparison of predictions and experimental data under Chinese mixed coal air combustion in boiler

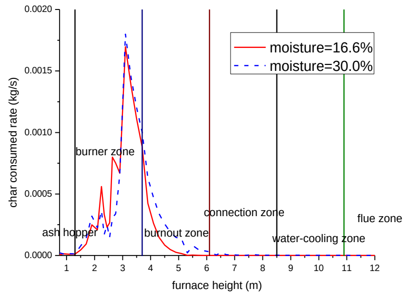
One of the important characteristics of Victorian brown coal is that it contains a lot of moisture. The Victorian brown coal flame pattern was studied in the 3MW boiler by modelling the conditions of different moisture contents. In order to achieve the same thermal power output compared to dry coal, it is necessary to burn more wet coals. The process conditions are shown in Table 4. The modelling results were illustrated in Figure 8. It's found increasing the moisture content within coal results in the expansion of the pulverized-coal flame length and char ignition delay.

**Table 4:** Modelling Cases of different moisture content for Victorian coal air combustion

| | | |
|---|---|---|
| Moisture as received (%) | 16.6 | 30.0 |
| Thermal power (MW) | 2.0 | 2.0 |
| Total coal flux (kg/h) | 334.87 | 407.88 |
| Excess air coefficient | 1.2 | 1.2 |
| Total primary air (Nm3/h) | 520.0 | 630.0 |
| Total secondary air (Nm3/h) | 1730.3 | 1670.5 |
| Ratio of solid-gas in primary air (kg/kg) | 0.5 | 0.5 |




(a) Gas temperature




(b) Char combustion rate

**Figure 8:** predictions of Victorian brown coal air combustion in boiler considering different moisture matter

The 3MW pilot scale boiler was retrofitted to research the oxy-fuel combustion of Victorian brown coal, by adding flue-gas recirculation pipeline. The system schematic is shown in Figure 9. The quantity of primary/secondary air and recycled flue gas can be calculated by the method written in the Appendix.

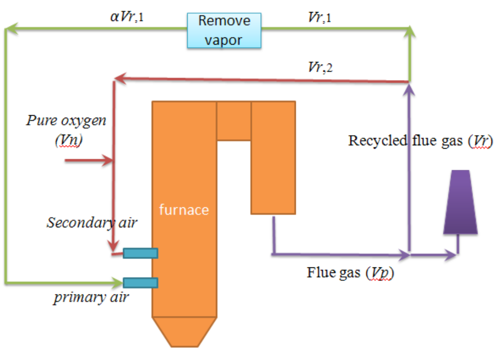



**Figure 9:** Schematic chart of oxy-fuel combustion system

Oxy-fuel combustion simulation has been conducted to study the influence of oxygen concentration in the flame. In oxy-fuel combustion, the concentration of oxygen in bulk gas is controlled by flue gas recycle ratio (See Table 5), which is also an effective measure to control the furnace temperature distribution.

**Table 5**: Simulation cases for the influence of oxygen concentration on oxy-fuel flame temperature

| | | | |
|---|---|---|---|
| Thermal power (MW) | | 2.0 | |
| Total coal flux (kg/h) | | 333.5 | |
| Excess air coefficient / | | 1.065 / | |
| New pure oxygen (Nm3/h) | | 439.7Nm3/h | |
| oxygen concentration in the flame | 21% | 27% | 30% |
| Flue gas recycled ratio | 80% | 71.6% | 67.9% |
| Total primary air (Nm3/h) | | 392.4 | |
| Total secondary air (Nm3/h) | 1966.1 | 1303.3 | 1090.3 |

The predicted results are shown in Figure 10. Increasing the oxygen concentration in bulk gas is essential to match the combustion temperature in air-firing case. Here again, it is further confirmed that achieving with a concentration of 27% for $O_2$ in circulated flue gas is essential to reach the identical particle temperature profile with that in air. Experiments are being conducted to validate this observation.

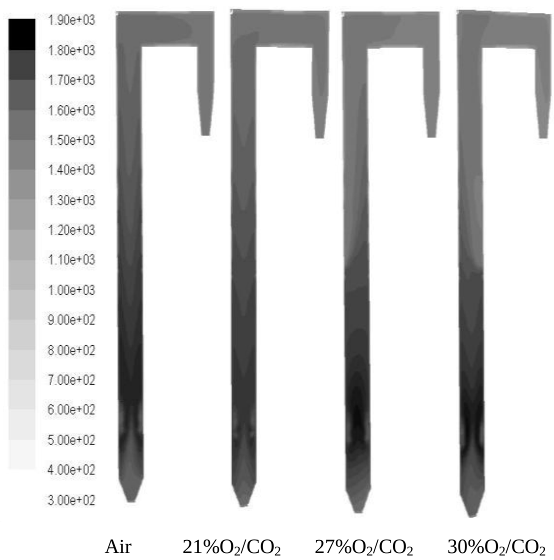



**Figure 10**: Prediction of different oxygen concentration in flame under air vs. oxy-fuel combustion in 3MW boiler

## CONCLUSION

In this study, a series of CFD modelling has been conducted by applying Ansys-Fluent to clarify the oxy-fuel combustion character of Victorian brown coal.

(1) From both lab-scale experiment and pilot-scale testing, it is clear that the use of 27vol% $O_2$ in recirculated flue gas is essential to match air combustion to achieve the identical particle temperature profile.

(2) For the combustion of Victorian brown coal, a larger amount of coal is required to achieve the same

thermal power as the dried coal, which results in the expansion of pulverized-coal flame length and char ignition delay.

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## APPENDIX

The oxy-fuel system flowsheet in figure 9 was established based on mass and elemental balance.

In calculation, the releases of nitrogen and sulfur from coal were not considered. The new pure oxygen flow is calculated as

$$V_n = \frac{V_{O_2,th}\varepsilon}{X_{n,O_2}} \tag{8}$$

Where $V_{O_2,th}$ is theoretical $O_2$ amount, $\varepsilon$ is excess pure $O_2$ parameter, $X_{n,O_2}$ is purity of pure oxygen.

The recycled flue gas stream is divided into two parts. The first stream is used to entrain coal particles. The second recycled gas stream is first mixed with pure oxygen and then entering furnace as secondary air. Hence the total recycle flue gas is

$$V_r = V_{r,1} + V_{r,2} \tag{9}$$

Then the secondary air is ($V_{r,2} + V_n$ ).

The solid-gas ratio (c) is usually set as 0.5 kg/kg in primary air. This configuration could keep the particles flow continuously into the furnace. Therefore total primary air flow is calculated as

$$\alpha V_{r,1} = \frac{m_{coal}}{c \cdot \rho} \tag{10}$$

Where $\rho$ is primary-gas density, $\alpha$ is a coefficient considering removed vapour. The Equation 11 can be derived from vapour mass balance.

$$\alpha = \frac{1 - X_{p,H2O}}{1 - X_{inlet,H2O}} \tag{11}$$

Where $X_{inlet,H2O}$ is volume fraction of water vapour in primary air, $X_{p,H2O}$ is volume fraction in produced flue gas . And $\alpha = 1$ means that no vapour removed.

Recycled ratio is defined as

$$re = \frac{V_r}{V_p} \tag{12}$$

The oxygen concentration entering furnace ( $X_{inlet,O2}$ ) could be set as 27%. On basis of mass balance of oxygen, then:

$$\beta = \frac{X_{in,O2} - X_{inlet,O2}}{X_{in,O2} - X_{p,O2}} = \frac{V_r}{V_n} \tag{13}$$

Besides above equation, the elemental balances of coal combustion are considered. So the flue gas composition and flow rates can be calculated.