REVIEW OF CFD SIMULATION OF OXY-COAL COMBUSTION FOR ELETRICAL POWER GENERATION: OPPORTUNITIES AND CHALLENGES

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ABSTRACT

The oxy-combustion has generated significant interested for reduction of CO_2 emission when the fossil fuel is coal, due to simplification on the separation process of CO_2 from the flue gas, it can be more easily stored in reservoir. The CFD numerical simulation techniques in oxy-coal combustion has the potential to contribute to designers in cost savings and reduced computational time; Furthermore, such techniques also provide a robust tool for better understanding and description of the aerothermodynamics processes involved, as well as, aiding the design of most efficient furnaces. However, to obtain representative results of the physical phenomena, the numerical models employed by CFD needs to be suitable for oxy-coal combustion. So, the aim of the paper is to carry out a review of the recent models that are being used for turbulence, combustion and pollutant emissions. Moreover, it is shown a comparison of different results obtained in the numerical simulation of oxy-coal combustion among new models, existing models and experiments. The analysis of the models and experiments shows that the challenges that are still being faced to obtain better accuracy of numerical simulation results. Improvements in the models for oxy-coal combustion can be seen like potential opportunities to investigate and optimize the process that occur in the combustion.

Keywords: oxy-fuel combustion, coal, CFD model

NOMENCLATURE

CFD	Computation Fluid Dynamics
DOM	Discrete Ordinates Method
LES	Large Eddy Simulations
PME	Process Model Environment
RANS	Reynolds Averaged Navier-Stokes
RFG	Recycled Flue Gas
RSM	Reynolds Stress Model
RTE	Radioactive Transfer Equation
TCI	Turbulence-Chemistry Interaction
TRI	Turbulence-Radiation Interaction
WSGGM	Weighted Sum of Gray Gases Model

INTRODUCTION

The demand for electricity is increasing and expected in near future to accounting for the greatest use of power for industrialized nations. In order to reduce greenhouse pollution emissions levels, the use of hydrocarbon fuels can be replaced with renewable resources, such as wind, solar, hydroelectric, wave/tidal, geothermal and biomass and biofuels. However, many of these technologies are still under development and unlikely to be able to reach in short time required low-carbon electric power. Fossil fuel power stations are the most flexible in terms of operational demands and the ability increase production when demand is high and crucial. Reduction of CO_2 emissions from coal fuel-fired power generation can be achieved by assumed advance technologies of carbon capture and storage such as oxyfuel combustion: the fossil fuel is burned in a mixture of oxygen and recycled flue gas (RFG). The resulting flue gas consists largely of water and CO_2. The conventional coal fuel-fired power stations use air as the oxidant, an oxy-fuel combustion plant uses an oxygen enriched gas, comprising oxygen, which has been separated from air, combined with RFG. The recycle moderates the too high flame temperature that would result from burning in pure oxygen. After removing water from the flue gas stream and removing trace pollutants, the result is high purity CO_2 and compressed for sequestration. The fundamentals of oxy-fuel combustion are shown in Fig. 1. The operational benefits are reduction of flue gas, reduction of heat loss from stream, improved combustibility and process flexibility, and a reduction of NO_x and SO_x emissions. The drawbacks are the increased operational cost of producing O_2 and compressing CO_2, that results in a less efficient process compared to air-firing.

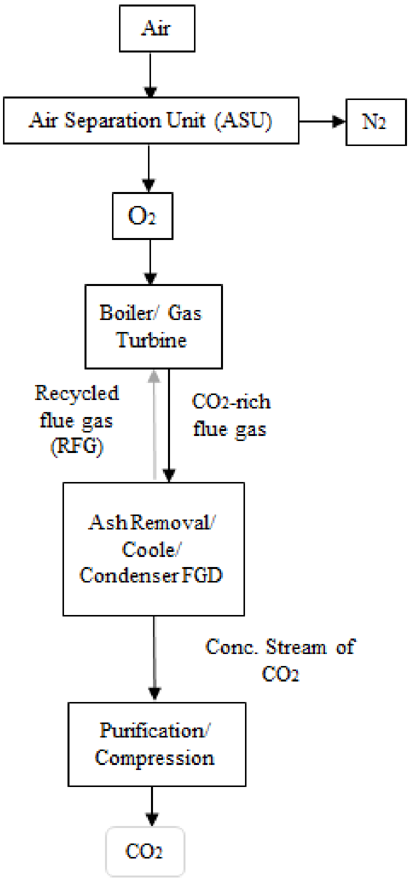

Figure 1. Fundamental of oxy-fuel combustion.

In 1980s, the pilot scale and demonstration plant studies were carried out by Argonne National Laboratories and the Energy and Environmental Research Corporation (Payne *et al.*, 1989; Abele *et al.*, 1987; Weller *et al.*, 1985). The corresponding numerical modelling investigations were carried out by Berry and Wolsky (1986) and Wang *et al.* (1988). During the 1990s, the technology received further interest for greenhouse gas and NO_x reduction with pilot-scale studies conducted by the International Flame Research Foundation (IFRF) (Woycenko *et al.*, 1995). Many reviews about oxy-coal combustion technology development have been presented (Wall *et al.*, 2009; Wall, 2005, 2007; Santos *et al.*, 2006; Croiset *et al.*, 2005; Kiga, 2001; Allam *et al.*, 2005; Buhre *et al.*, 2005; Jordal *et al.*, 2004; Toftegaard *et al.*, 2010). These reviews give details of the progress and understanding obtained from experimental and pilot-scale facilities and the application of mathematical models for the processes is less progressed and has therefore received less attention.

Computation fluid dynamics (CFD) modelling is used as part of a design tool for oxy-coal combustion. The combustion process can be modelled in 3D and the overall impact of changing design parameters such as burner configuration, or combustion environment can be investigated by the CFD technology. The aim of the paper is to carry out a review of the recent models that are being used for turbulence, combustion and pollutant emissions. Moreover, it is shown a comparison of different results obtained in the numerical simulation of oxy-coal combustion among new models, existing models and experiments. The analysis of the models and experiments shows that the challenges that are still being faced to obtain better accuracy of numerical simulation results. Improvements in the models for oxy-coal combustion can be seen like potential opportunities to investigate and optimize the process that occur in the combustion.

CFD MODELLINGS OF OXY-COAL COMBUSTIONS

The simulation with CFD needs accurate sub-models to describe devolatilisation, char combustion, pollutant formation and extinction and heat transfer for turbulence and the interactions between turbulence with chemistry and heat transfer. Some of models require significant adaptation before being reliably used to oxy-coal combustion. Turbulence impacts combustion from heat transfer to chemical kinetics. The fundamental equations for conservation of mass, momentum and energy, and species transport are solved in CFD tools (Versteeg and Malalasekera, 1995). In order to simplify, the effects of gravity can be neglected and an inertial reference frame assumed. The governing equations cannot be solved by analytical methods and so numerical discretization is used. Many available methods including Finite difference (Forsythe and Wasow, 1960), Finite Elements (Zienkiewicz *et al.*, 2005), Orthogonal Collocation on Finite Elements (Carey and Finlayson, 1975), Spectral methods (Gottlieb and Orszag, 1977), Finite Volume discretization (Versteeg and Malalasekera, 1995) are commonly employed in computational fluid dynamics codes. This allows representing the complex geometries of burners layouts on which physical phenomena are occurring. Usually non-uniform grid is necessary and the good solution depends on the quality of the grid and order of the discretization method. Modelling of solid coal introduces additional complexities as the solid has highly different transport properties from the surrounding gas. The most common approach is to treat the solid and fluid phases separately and couple them by the use of appropriate source terms. For that, two assumptions are made: the solid particles have a negligible volume compared to the fluid (it is invalid close to the burner where coal particles are concentrated in a small area and inclusion of a particle collision model is required), and the particles are adequately dispersed so collisions are not encountered. The following is made a discussion about turbulence models.

Turbulence Flow and Heat Transfer

To calculate the turbulence, turbulence model is necessary to close the time-averaged Reynolds Averaged Navier- Stokes (RANS) equations. The appropriate RANS model depends on the characteristics and geometry of the flow and the computational efficiency. There are three main types of RANS models, **linear eddy-viscosity models, non-linear eddy-viscosity models and Reynolds Stress models (RSM).**

The linear eddy-viscosity models assume isotropy of the Reynolds stresses and link them to a scalar eddy viscosity, usually via a time and length scale, which are calculated by solving transport equations. For combustion flow, at least two-equations are required in order to have independent calculation of the turbulent viscosity and length scale. Models commonly incorporated into commercial CFD codes include the k–ε model (Launder and Spalding, 1972), k–ω model (Wilcox, 1998) and Shear stress transport model (Menter, 1994). For combustion flow prediction, RANS modelling of turbulence is given by Launder *et al.* (1975), Lien and Leschziner (1994), Wilcox (1998) and Batten *et al.* (2000).

- The standard k–ε model is well known and has several adaptations, which are suitable for certain combustion flow. The k–ε variant (Batten *et al.*, 2000) has basic foundation for the dissipation rate and variable model constants, which ensure physical laws are not broken. These variants have been used extensively in combustion (Fan *et al.*, 2001; Edge *et al.*, 2011a). None model has been shown to consistently outperform the others and so the model selection should be made on a case-by-case basis.
- The k–ω model solves for ε/k instead of the dissipation rate ε, and includes low-Reynolds number correction in the model constants. The advantage of it is applicable throughout the boundary layer, if near-wall meshing is sufficiently fine, and empirical wall functions are not required. The limitation of this model is that conversely it performs less well in free flows. As noted by Spalart (2000), free-stream behavior is usually much more important than the wall limit. Menter (1994) recognized this and developed a hybrid 2-equation model, which behaves like k–ω in near-wall regions and k–ε in free flows, with a blending function applied in the boundary layer.

Non-linear eddy viscosity models relax the Boussinesq hypothesis (Hinze, 1975), and allow for anisotropy of the Reynolds stresses. It is analogous to the algebraic stress model (Gatski and Speziale, 1993). The computational requirement is in-between that of linear eddy-viscosity models and RSM. However, diffusion effects are potentially important in inhomogeneous media and thus this approximation is questionable for oxy-coal combustion.

The Reynolds stress model (RSM) (Launder *et al.*, 1975) solves the transport equations for the Reynolds stresses in addition to k-ε, resulting in 7 equations for 3D cases. Gran *et al.* (1997) have reported improvement in reproductions of observed flow patterns in the near burner region for combusting flow using RSM. Breussin *et al.* (1996), found that the RSM improved NO_X predictions compared to k–ε models. Lockwood and Shen (1994), found RSM to predict flames that were too short and intensive.

The models limitation is the empirical or semi-empirical transport equation for the scalar dissipation rate, ε, which is the source of uncertainty and controversy over 2-equation and higher order models (Wilcox, 1988). Near to the burner zone, the flow has very complicated flow patterns including high levels of swirl and internal recirculation. Pollutants Accuracy predictions in such flows typically cannot be achieved using Reynolds-averaged Navier–Stokes (RANS) simulations (Pitsch, 2006). An alternative technique to averaging is to filter the flow variables. Turbulent flow is composed of a spectrum of energy carrying eddies (Kolmogorov, 1941 and Oboukhov, 1961). The Large Eddy Simulations (LES), a filter is used in order to separate the large eddies from the small eddies. The filtering can be done by wave number (Sharp filter/low pass filtering, Frisch, 1995). For good LES, it is recommended that the majority of the inertial scales should be resolved in order to accurately capture the spectrum (Edge et al., 2011a).

Frisch (1995) linked the energy spectrum to the Reynolds number and suggests a suitable spacing of $Re^{9/4}$ grid points per integral length scale in order to fully resolve the inertial scales. The time step used should be proportional to the mesh spacing. After the application of the filter, the “large eddies” are resolved, and the “small eddies” have to be modelled. This saves a great amount of effort compared to resolving the full spectrum, but is still time-consuming than RANS modelling as time-dependency is considered.

LES has been widely applied to gaseous and spray flames but only a few cases have been reported for pulverized fuel systems, considering either no combustion or the near-burner resolution (Smith *et al.*, 2008; Reid *et al.*, 2009; Stein and Kempf, 2009).

The major challenges of LES applied to coal are: computational requirement and particle treatment. Good grid spacing may be computationally prohibitive as Reynolds numbers in coal flames can range from 10^3 to 10^5, and integral length scales range from 10^{-4} to 10 m.

The particles can be treated in a Lagrangian reference frame and coupled to the gas phase as with RANS models and the particle should be related to the LES time-step. In pulverized fuel RANS models, the flow-field is first solved, then the particles are injected and then the flow-field is recalculated to include the effects of the combusting particles. This procedure can be carried out for every time-step, however to reduce the computational requirement it may be possible to inject the particles every 10 or 20 time steps, after an initial flame has been generated. There is also an additional limitation on the potential improvements of LES over RANS.

In pulverized fuel combustion, the chemical reaction rate, LES has been shown to predict the scalar mixing process and dissipation rates better than RANS in chemistry predictions (Pitsch, 2006). The turbulence treatment determines the depth and type of information available on the flow and the suitability of other sub-models. Most of sub-models were developed for RANS. The challenge for LES is to take advantage of knowledge of the resolved scales, for example, similarity models (Veynante, 2005).

LES can offer additional information on pulverized fuel combusting flows in terms of the flame intermittency and stability effects. Accurate modelling of flame stability is desirable since experimental studies have suggested CO_2 has an inhibitory effect on flame stability for oxyfuel combustion (Buhre *et al*., 2005). LES can be used for stability by generating flame animations and by calculating the flicker frequency. Hence, LES could model pollutants in the exhaust gases more accurately than RANS.

Interaction and Simulation

Accurate solutions to modelling of combustion characteristics are only achievable if good predictions of heat transfer can be achieved. In air and oxy-coal combustion the dominant mode of heat transfer is by radiation because of the high temperatures within the flame zone. To calculate radiation within a utility boiler the radiative transfer equation (RTE) must be solved and coupled with a radiative properties model that specifies the gaseous and particle properties. The RTE describes mathematically an energy balance on an elementary volume taken along the direction of a pencil of rays within a certain elemental solid angle (Viskanta and Mengüc, 1987). Comprehensive reviews that describe the different methods for solving the RTE were done by Viskanta and Mengüc (1987) and Modest (2003). The principal solvers usually considered for solving the RTE include the discrete ordinates method (DOM), spherical harmonics (P1) method, the discrete transfer ray tracing method, and the Monte Carlo method (Edge *et al*., 2011a). The P1 method is easily compatible with CFD and has very fast computation times, but has reduced accuracy due to modelling assumptions and should be used only in certain cases. P1 method is often considered appropriate for use in air firing and the optical thickness increases in oxy-coal combustion and therefore it can also be used for oxy-fuel with more confidence.

Accurately model heat transfer in CFD models of combustion is vital because correct temperature profiles can only be predicted with accurate radiation determination and chemical reaction rates are directly related to temperature. Heat transfer cannot be separated from other physical processes including turbulence and chemical reactions. Recent developments in spectral models for oxy-fuel in CFD have been focused on utilizing global models, because constraints on computational resources means that band models are prohibited for CFD. Band models are also only compatible with ray tracing methods meaning that the majority of RTE solvers in CFD cannot be used. In CFD, ray tracing methods rely on pre-processing that may neglect some aspects of the particle effects, which is undesirable in oxy-coal combustion. Edge *et al.* (2011a) have reported many approaches to take into account the radiation effects for CFD simulation.

There are two challenges to overcome, one is the incorporation of non-gray models for oxy-coal combustion in CFD that are concentrated on computational time and integration with RTE solvers. It is essential to ensure that models are compatible. Other challenge is the integration of the gaseous model with the particulate absorption and emission model in oxy-coal, because not all models will allow for scattering and absorption by particles.

Turbulence–chemistry interaction (TCI) is modelled mathematically using the following methods depending on the nature of the combustion and flame. There is no universal model that is applicable to oxy-coal combustion and it depends largely on the case considered. Laminar flamelet models (Peters, 1986; Bray and Peters, 1994) assume that turbulent diffusion flames consist of a large number of quasi-steady one dimensional laminar diffusion flames. This model is very complex in practice and computationally intensive. Eddy Break Up model (Spalding, 1970) assumes that the rate of consumption of fuel is specified as a function of local flow properties and the mixing process only controls reaction rates. Due to the dependence of the fuel dissipation rate on the turbulence time scale, the quality of predictions is highly dependent on the performance of the turbulent model. A modified version of Eddy Break Up is known as Eddy Dissipation Concept (Magnussen and Hjertager, 1976; Magnussen, 1981). This model incorporates the significance of good structures in a turbulent reacting flow in which combustion chemistry is important. This model is used to all types of fossil fuel combustion and is relatively simple to use.

As with many aspects of combustion modelling in CFD, radiation and turbulence are not independent physical processes with each having significant impacts on the other as mentioned before. Turbulence–radiation interactions (TRI) are the interactions between the flow and radiation fluctuations. Due to computational limitations and difficulties in solving the complex closure equations required to model TRI effects, it has been neglected in computations of combusting flows, and radiation and turbulence have been treated separately. The modelling of TRI in oxy-coal combustion should not be fundamentally different from air combustion, because the same physical processes of radiation and turbulence are being modelled. In oxy-coal combustion, gases are optically thicker and the impact of this on the relative importance of absorption TRI over emission. TRI is a challenge that should be examined.

In general, simulation tools are very fast but as a result their generality and accuracy can become compromised, as they are often fine-tuned to specific environments. It is desirable to investigate integration of oxy-coal plant components within a Process Model Environment (PME). For extensive investigation and optimization of oxy-coal technology, the direct integration of CFD with various process simulation tools is recommended. CFD techniques are used to account for the complex chemistry and heat transfer phenomena in the furnace, which are very much affected by the physical change from conventional air-firing to oxy- coal combustion. A general framework for co-simulation of chemical and energy processes via CFD-PME has been described by Bezzo *et al.* (2000). It shows a good tool for power plant retrofitting what is interesting for Brazilian existing Power Plants, using national coal.

Kinetics Modellings of Coal Combustion

Most of the existing models for char combustion are done for conventional combustion therefore needs to incorporate the gasification reaction and the thermal gas properties to have better accuracy results of oxy-coal combustion. At the time, exist models that simulate the NO_X in an oxy-coal combustion, but these models can be improved. Other studies were carried out to predict the sulphur gas during the oxy-combustion of lignite (Edge *et al.*, 2011a). It was seen that the SO_3 in oxy-combustion was four times greater than conventional, being necessary some adjust, as measure, to accurate the model (Fleig *et al.*, 2009). Have a few works done about emission of mercury. A study about emission of mercury said it is not affected in a medium of O_2/CO_2, when the model does not consider the effect of recirculation (Zheng e Furimsky, 2003). Soot models are considered secondary importance in a furnace reaction, which have others major pollutants inside it, as SO_X and NO_X. The models used in soot are the same as conventional but with different constant because of distinct reactions (Edge *et al.*, 2011a).

VALIDATION

This section will show the validation of some works for CFD models made of oxy-coal combustion with tests carried out in laboratories, and the discussion of its results, the benefits and challenges that the models can get to simulate this new combustion technology used for coal.

Edge *et al.* (2011b) compared the numerical simulation using the LES with the RANS in CFD of the conventional pulverized coal combustion and oxy-coal combustion, and tests made on 0.5 MWth RWEn power. The simulations were effected in two furnaces using also two different bituminous coals. The non-gray radiation method was considered in order to cope with the spectral absorption and emission nature of the oxy-coal products. Three tests were made. In the first case, was used the turbulent RNG k-ε model and the other two cases used the standard k-ε model, which 1st and 2nd case was air-firing and 3rd case was used oxy-fuel. In all cases investigated in the radiation process, the weighted sum of gray gases model (WSGGM) was coupled with the DOM.

The results suggested that LES model get a better simulation of recirculation zone and flame configuration, and demonstrates the importance of the radioactive properties of the gas. In the combustor exit, comparing the temperature values obtained by LES, RANS and the experimental data, Tab. 1, it is observed that the results from LES are more approached the trial data. Regarding radiation incidence, in the IFRF furnace, there was a difficulty to reproduce the real case because the model neglects the effects of decoupling.

Table 1. Exit Temperature of the combustion test facility (Edge *et al.*, 2011b).

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

A work done by Hu and Yan (2013), investigated by numerical simulation, using the CFD ANSYS FLUENT 13.0, models of the effects of absorption coefficient and the radiation intensity in the oxy-coal combustion with RFG or conventional combustion. The analysis has as parameters the relationship between the ratio of RFG and the O_2 concentration in various conditions. It was used to study the radiation intensity on the sidewalls. These results are validated with a test done in a 0.5 MW RWEn power combustion test facility.

The models used in numerical simulation, were for discrete phase (coal particles) the model of Eulerian-Lagrangian approach; SIMPLE algorithm for coupling the speed and pressure; the k-ε turbulence model; in the volatile combustion it was used finite-rate chemistry /eddy-dissipation model; the char combustion model is given by the chemical kinetic rate and external diffusion rate of oxygen to the char surface; the DOM and two models of WSGGM (Yin and Smith) are used to the radiation model.

The WSGGM-Yin model has the best result of surface incident radiation (kW/m^2), as seen in Fig. 2, but the model with the constant absorption coefficient can be seen a practical way in the engineering in which provides acceptable results with a much lower computational effort. Al-Abbas *et al.* (2011), which compared the model of the absorption in CFD with laboratory experimental data, carried out the finding of this values difference in the oxy-coal combustion. However the use of this model for applications in large scale (such as industrial combustion chamber) should be studied due to the deviation in the total emissivity grow with the beam length. Another factor observed is that when the O_2 concentration is greater than 29%, in oxy-coal combustion, the incident radiation on the upstream surface of the combustor is greater than conventional and thus can reduce their area at the entrance.

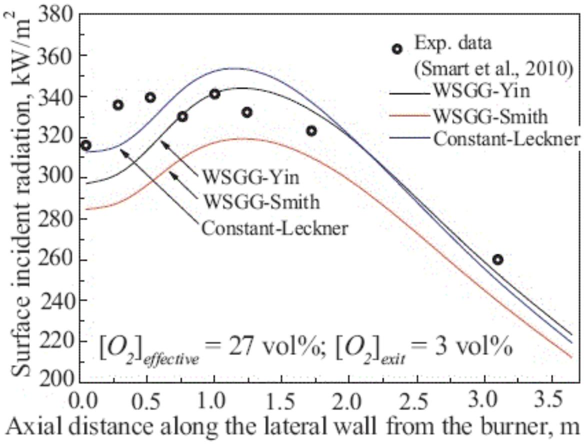

Figure 2. Surface incident radiation calculated with specific absorption coefficient model (Hu and Yan, 2013).

CONCLUSIONS

A review of the recent models that are being used for CFD simulation and validation has been carried out and the main opportunities and challenges surrounding the development of computer based models for the oxy-coal combustion process are shown as follow.

The heat transfer and kinetics have a great impact on CFD simulation of oxy-coal combustion and for that an accurate model is required. The linear eddy viscosity models can be used if a reasonable compromise between accuracy and computational efforts. Existing models can cope with oxy-coal combustion since very carefully section of the models is done.

The non-gray radiative properties of the combustion gases cannot be neglected in oxy-combustion that because of radiative heat transfer is very different from air combustion. Appropriate model should be selected to represent it. The accurate models can predict the radiative heat fluxes and temperatures, which is essential for modelling oxy-coal combustion. Challenges in introducing a computationally efficient non-gray model for radiation and linking this with various types of RTE solvers are opportunity for further research and development. The improvement in WSGGM has shown to be a good method because of its simplicity and accuracy.

The validation is a mechanism used to ensure that the numerical simulation is similar to what actually occurs in the nature. To show the effects that happen in oxy-coal combustion the CFD package needs to be validated with a test data. Hence, the need for accurate oxy-combustion models so there is a good characterization of the chemical process.

Currently available models for TCI and TRI do not require modification for oxy-fuel combustion. On the other hand, application of detailed models is currently prohibited due to the high computational requirements. One of the opportunities in researches is the improvement on TCI and TRI that will have an effect on the accuracy.

System simulation is vital to perform accurate techno-economic evaluations of oxy-coal technology for new power plant design and retrofitting of existing coal power plant. A general framework for co-simulation of chemical and energy processes via CFD-PME has been used as good tool for power plant retrofitting what is interesting for Brazilian existing Power Plants, using national coal.

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RESPONSIBILITY

The authors are the only responsible for the printed material included in this paper.