2nd Oxyfuel Combustion Conference

Comparison of RANS and LES Turbulence Models for Predicting Air-coal and Oxy-coal Combustion Behaviours

D. Caridi[a], D. Couling[b], M. Gharebaghi[c], S.R. Gubba[c], R.M.A. Irons[b], L. Ma[c], M. Pourkashanian[c], A. Pranzitelli[c,*] and A. Williams[c]

[a]*ANSYS UK Ltd., Sheffield S9 1XH, United Kingdom*
[b]*E.ON New Build and Technology, Technology Centre, Ratcliffe-on-Soar, Nottingham NG11 0EE, United Kingdom*
[c] *CFD Centre, School of Process, Environmental and Materials Engineering, University of Leeds, Leeds LS2 9JT, United Kingdom*

Abstract:

It is commonly accepted that with existing physical sub-models, computational fluid dynamics (CFD) can offer significant insight to the complex combustion systems such as those found in the coal-fired power generation industry. With the growth of computing resources and, in particular, the availability of powerful computer clusters, application of Large Eddy Simulation (LES) emerges as an attractive option in modelling of turbulence combustions in coal-fired furnaces. This paper presents the results from a CFD simulation of the coal combustion processes, under both air-fired and oxy-fired conditions in a 1 MW_{th} industrial combustion test facility. Both Reynolds Averaged Navier–Stokes (RANS) and LES approaches have been employed and the results are compared with each other and with experimental measurements. Advantages of the LES underlining its potential for future industrial applications are addressed. It is shown that validation a CFD model that is based on LES requires more detailed experimental data from well-controlled experimental measurements.

Keywords: **Coal Combustion, CCS, CFD, LES**

1. Introduction

Oxy-coal combustion with recycled flue gas is one of the candidate technologies that offer the prospect of significantly reducing CO_2 emissions to the atmosphere. In oxy-coal combustion, the recycled flue gas moderates the high flame temperature resulting from the combustion of coal in oxygen-enriched environment. However, elevated concentration of the combustion products and low content of nitrogen have important implication for the combustion chemistry and flow dynamics. Differences in nitrogen and CO_2 thermo-chemical properties, lead to different flow rates, heat transfer pattern and flue gas speciation.

Computational fluid dynamics (CFD) has been acknowledged as a useful design tool for many years in engineering applications [1-3]. Recent developments in computer resources and numerical techniques, which contribute to fast and cost-efficient data processing and grid generation, facilitate CFD with more reliability and accuracy. Among various physical sub-models used in CFD modelling of coal combustion, turbulence is a topic of considerable importance in mechanical engineering and study of the flow.

For fluid flow simulation, steady state RANS (Reynolds-Averaged Navier-Stokes) calculations are commonly used in engineering practices. The reason is the reasonable computational costs and acceptable accuracy of the

* Corresponding author, Tel.: +44 (0) 113 343 2481; fax: +44 (0) 113 246 7310.
E-mail address: a.pranzitelli@leeds.ac.uk.

predictions. However in the past decade, with the continuing increase in speed and memory of computers, Large-Eddy Simulation (LES) has begun to play a significant role in understanding and predicting turbulent reacting flows. Riley [4] has reviewed LES performances in non-premixed turbulent combustion simulations. By highlighting the importance of the sub-grid scale model selection and the effect of chemistry, he suggested that LES can now confidently be applied to problems with "mixed is burnt" assumptions. Sadiki et al [5] have assessed the capabilities of unsteady RANS and LES for the simulation of gas combustion systems and have concluded that when appropriate choices of boundary and inflow conditions are made, a good predictability could be achieved from LES. However, very few studies on the application of LES for coal combustion simulations, involving pulverized coal particles are reported [6]. Handling heterogeneous combustion including particles would require more efficient LES codes and enhanced computational resources.
In this study, application of RANS and LES turbulence models for the prediction of the behaviour of the pulverized coal particles in a 1 MW_{th} test facility has been established. Extra attention has been paid to the grid generation and optimization processes.

2. Experimental Setup

The data from a 1 MW_{th} combustion test facility (CTF), located in Ratcliffe–on–Soar, United Kingdom are used for model validation. The CTF has been simulated in previous studies by the authors [1, 7] and has been selected because its level of complexity is simpler than a complete power generation furnace but allows simulation of the key processes that may be found in a full-scale industrial boiler. Measurement data include the exhaust gas temperature and species concentrations within the furnace and the convection duct. Inlet oxidizer velocity, temperature and fuel flow rate are monitored. The test facility is equipped with a single wall-fired low NO_x burner which is a swirl-staged type with variable swirl. More details on the CTF can be found in [7].

3. Grid Generation/Optimization

The furnace including the burner is modelled in full 3D, giving a total cell count of approximately 3 million. Even though tetrahedral meshes are easy and time-efficient to construct in complicated geometries such as burners with vanes, an unstructured grid, made mostly from hexahedral cells, has been preferred to reduce the numerical diffusivity. Due to its complexity in the geometry of the CTF around the burner, a small amount of polyhedral cells has been used in the burner. The grid has been used for both RANS and LES simulations. Calculations prior to grid generation have been performed in order to estimate the turbulence integral length scale of the fluid flow and it is indicated that the mesh used in this study is fine enough for carrying out LES simulations. Figure 1 shows the cell distribution in central plane of the CTF, a 3D mesh and a schematic of the burner.

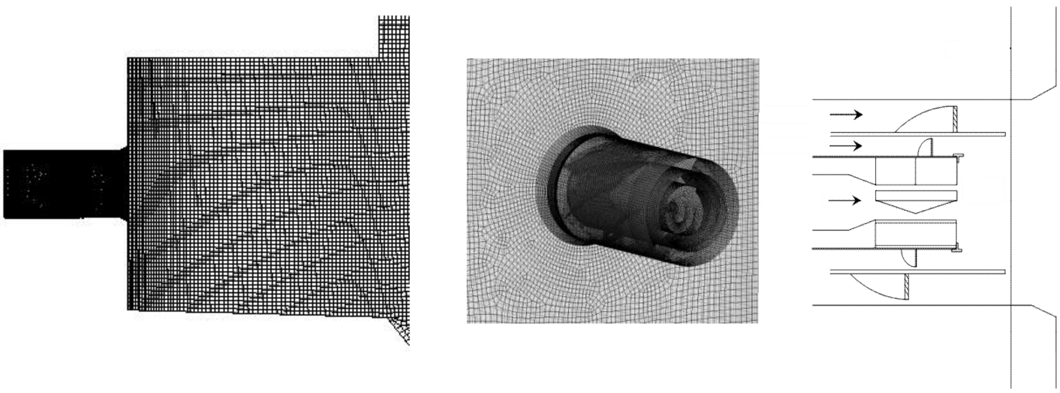


Figure 1: details of the grid and burner cross section

4. Computational Approach / CFD Physical Sub-models

Air-coal and oxy-coal combustion have been modelled and the predictions are validated with the available experimental data. The RANS solution of each case has been used as initial condition for the respective LES case. It should be borne in mind that LES calculations should be validated with well-controlled and more detailed measurements. Table 1 shows the operating and boundary conditions for air-coal and oxy-coal combustion.

Table 1: Operating conditions of the test cases

	Air-coal combustion		Oxy-coal Combustion	
	Flow rate (kg/h)	Temperature (K)	Flow rate (kg/h)	Temperature (K)
Coal	131.5	353	146.3	353
Primary	260	353	183	353
Secondary	1120	563	1033	509

4.1. RANS Simulations

Thoresby (British bituminous coal) is used for these calculations. Coal analyses have been given in Ref [7]. The numerical modelling has been carried out by utilizing commercial CFD code, ANSYS Fluent V. 12.1. As for the fluid flow prediction, velocity-pressure coupling is handled through SIMPLE algorithm, and the turbulence is modelled by the standard k-ε model. Thermal model includes radiative heat transfer modelling using the Discrete Ordinate (DO) model and the WSGGM have been considered for the absorption coefficient of the gas mixture. Transport equations for the gas phase are solved using Eulerian approach and particles are tracked in Lagrangian frame of reference across the flow field. Single kinetic rate devolatilisation model has been employed based on the available information for Thoresby. Char combustion is simulated using intrinsic model and volatile combustion is calculated with a two-step global reaction mechanism. Turbulence-Chemistry Interaction in the gas phase is modelled using Eddy Dissipation Model (EDM). Second order upwind scheme is used to solve momentum, energy and species transport equations. The convergence criteria are set with residuals for the momentum equation less than 10^{-4} and scalar equations less than 10^{-6}.

4.2. LES Simulations

ANSYS Fluent solves the strongly coupled Favre-filtered flow equations outlined in the above sections. All solid wall boundary conditions are applied with the power-law wall function of Werner and Wengle [8] for the calculation of the wall shear stresses. The second order bounded central differencing scheme is employed for the momentum equation in the LES, while second order upwind scheme is used for species and energy. The first order upwind scheme is used for radiation equations and the equations are advanced in time using the second order implicit scheme. A number of iterations are required at every time step due to strong coupling of equations with one another. Extra care has been taken to simulate the particle phase for every time step of the continuous phase simulation. The convergence criteria is set to be at each time step with residuals for the momentum equation less than 10^{-3} and scalar equations less than 10^{-6}. A small time step of 5×10^{-4} s is chosen to advance the LES solution.

The simulations have been performed on a computer cluster using 30 processors. One second of the combustion time requires about 15 days of computational time.

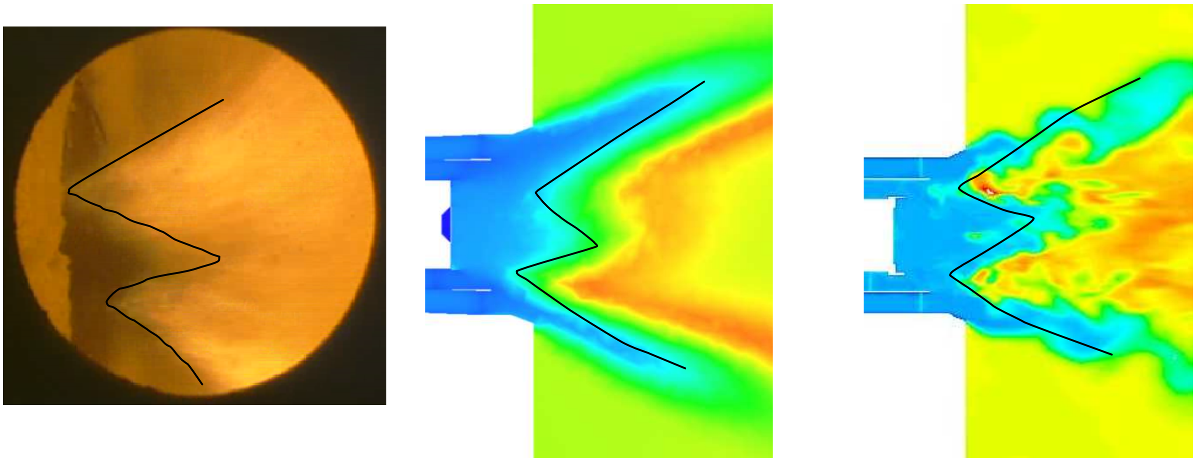
5. Results and Discussion

Figure 2 shows the comparison between an extracted image from the flame video (Fig.2a), the temperature contours from the RANS calculations or averaged values (Fig.2b) and the instantaneous values from LES computations (Fig.2c) at the central plane of the CTF under air-coal combustion conditions. It is noted that the temperature contours obtained from the LES are qualitatively in agreement with the global flame structure shown in Fig. 2a. The preheated region showed upstream of “w” shape in Fig. 2b and 2c before main flame is also predicted very well and in agreement with the image showed in Fig. 2a. Attempts have been made to validate the selected physical models in Ref. [6]. Note that in order to have accurate predictions from both RANS and LES simulations, there is a need for isolated and well-controlled measurements of the flame speed, temperatures and major species in the flame region and afterwards.

6. Conclusion and Way Forward

In this study, RANS and LES simulations of air-coal and oxy-coal combustions in a 1 MWth combustion test facility have been performed. It has been found that by using a high quality and optimized grid, predictions from

LES simulation are in good agreement with flame shape monitored at the facility. With the fast growing of computational resources, it is believed that once coupled with improved radiation and chemistry models, LES approach can also be used for prediction of flame stability, shape and speed in oxy-coal combustion.



(a) (b) (c)

Figure 2: Comparison of temperature predictions with experimental data, a) image extracted from flame video, b) RANS static temperature contours at the vertical mid plane, c) instantaneous temperature contours at the vertical mid plane. Temperatures are in K.

7. Acknowledgement

Financial support from E.ON Engineering UK, EPSRC, Dorothy Hodgkin Postgraduate Awards and OXYCap-UK is gratefully acknowledged.

8. References

[1] Edge, P., Gharebaghi, M., Irons, R., Porter, R., Porter, R.T.J., Pourkashanian, M., Smith, D., Stephenson, P. and Williams, A., *Combustion modelling opportunities and challenges for oxy-coal carbon capture technology*, Chem. Eng. Res. Des., [In Press]

[2] Backreedy, R.I., Fletcher, L.M., Ma, L., Pourkashanian, M. and Williams, A., *Modelling pulverised coal combustion using a detailed coal combustion model.* Combust. Sci. Technol., 2006 178: p. 763-787.

[3] Pallares, J., I. Arauzo, and A. Williams, *Integration of CFD codes and advanced combustion models for quantitative burnout determination.* Fuel, 2007 86(15): p. 2283-2290.

[4] Riley, J.J., *Review of Large Eddy simulation of Non-premixed turbulent combustion.* Journal of Fluid Engineering, 2006 128: p. 209-215.

[5] Sadiki, A., Maltsev, A., Wegner, B., Flemming, B., Kempf, A. and Janicka, J., *Unsteady methods (URANS and LES) for simulation of combustion systems,* International Journal of Thermal Sciences, 2006 45(8): p. 760-773.

[6] Edge, P., Gubba, S.R., Ma, L., Porter, R., Pourkashanian, M. and Williams, A., *LES modelling of air and oxy-fuel pulverised coal combustion–impact on flame properties*, Proc. Combust. Inst., 33 (2011) 2709-2716.

[7] Gharebaghi, M., Goh, B., Jones, J.M., Ma,L., Pourkashanian, M. and Williams, A. *Numerical Investigation of Char Reactivity in Oxy-coal Combustion in Carbon Capture and Sequestration Technolgies* in *ASME-Turbo Expo*. 2009. Orlando.

[8] H. Werner, and H. Wengle, *Large-eddy simulation of turbulent flow over and around a cube in a plate channel*, 8th Symposium on Turbulent Shear Flows Munich, Germany, 1991.