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Towards Large Eddy Simulations of a Bluff Body Burner Using an Unstructured Grid

Shafiq R. Qureshi*and Robert Prosser†

Abstract—**A Large Eddy Simulation of a bluff body flame has been carried out using an unstructured grid. The flame, burning a methane-hydrogen fuel with detailed combustion chemistry (based on a mechanism of 18 species) is simulated using STAR-CD. The mixture fraction is used as a conserved scalar, and a subsequently temperature, density and species mass fraction are calculated using a probability density function. A beta function presumed-PDF (PPDF) has been used. The beta function is parameterized by the filtered mixture fraction and mixture fraction variance. The Scalar dissipation is modeled by assuming proportionality between the sub grid mixing time scale and turbulent time scale. Due to the large domain size, the adequate resolution of the reacting part of the flow presents a challenge. To address this difficulty, we have exploited embedded mesh refinement in and around the reaction zone. The velocity profiles are in good agreement near the jet inlet but are slightly over predicted at the center line, far from the jet inlet. The model has under predicted the temperature at the start of the flame. The selection of a correct coefficient for the scalar dissipation is identified as the source of the under prediction.**

Keywords: LES, Combustion, PPDF, Unstructured grid, Subgrid Model

1 Introduction

Turbulent combustion is encountered in many applications such as piston engines, gas turbines and industrial gas burners[1]. The development of modern computational methods have led to an improved predictive capability for turbulent reactive flows. We can delineate between three separate approaches - DNS, LES and RANS. Direct Numerical Simulation (DNS) of large flow domains is yet not possible due to the large computational requirement. DNS requires the number of grid points to scale as $Re^{9/4}$, where Re is the Reynolds number [2]. For this reason DNS is limited to very simple geometries,with low values of Re. Its application to practical engineering problems is unlikely in near future. RANS approaches have been in use for quite a long time for flow simulation. Because only average statistics are captured (with no detailed information of instantaneous quantities), RANS models do not provide information on the wave number and frequency distribution of the turbulent eddies [3]. Large Eddy Simulation (LES) is an intermediate approach, which solves the dynamics of the large eddies while modeling the small subgrid scales. LES has become a powerful and promising tool for simulations, overcoming many limitations of RANS approaches.

In combustion simulations, the reaction physics needs a description along with other turbulent properties of the flow. The chemical reactions in combustion occur at very small scales (smaller than the turbulent scales). The accurate simulation of the combustion process still poses a challenge for the CFD community [4].In the case of non reacting flows, most of the kinetic and scalar energy is resolved by solving the momentum equation and the scalar equation at large scales; subgrid models are only required to extract the correct amount of energy from the large scales. However for the case of reacting flows, this concept cannot work because the evolution of reacting scalars (i.e. chemical species) rely upon turbulent mixing and molecular diffusion. The rate of reaction is often controlled by the rate of mixing [5].The time and length scales related to reaction dynamics are very small and the major portion of these processes lies in subgrid scales. A presumed probability density function(PPDF) has been implemented by numerous authors [6],[7],[8] and is considered as an accurate and practical approach to capture the subgrid dynamics of reacting flows.

In Section 2 the mathematical model for the LES and the treatment of the subgrid scalar variance is briefly discussed. Section 3 describes the configuration of the bluff body flame used for the simulation. The comparison of the results with experimental data are discussed in Section 4.

2 Mathematical Models for LES

In Large Eddy Simulation, a filtering operation is applied to the governing transport equations to remove the scales smaller than a characteristic width [9]. In this way only the large scales of motion are resolved. The energy dissipation at smaller scales is accounted for with subgrid scale (SGS) modeling. Here, the Smagorinsky model is used for subgrid scale modeling. The filtering operation

*University of Manchester, School of MACE. Email: s.qureshi@postgrad.manchester.ac.uk
†University of Manchester, School of MACE. Email: robert.prosser@manchester.ac.uk

can be defined as [9]:

$$\overline{U}(x,t) = \int G(r,x)U(x-r,t)\mathrm{d}r \tag{1}$$

Where the filter G satisfies the condition:

$$\int G(r,x)U(x-r,t)\mathrm{d}r = 1. \tag{2}$$

The resultant filtered transport equations can be written in the form [10]:

$$\frac{\partial \overline{u_i}}{\partial t} + \frac{\partial \overline{u_i u_j}}{\partial x_j} = \frac{\partial \overline{p}}{\partial \overline{x_i}} + 2\frac{\partial}{\partial x_j}[(\nu+\nu_T)\overline{S}_{ij}] \tag{3}$$

$$\frac{\partial \overline{Z}}{\partial t} + \overline{u_j}\frac{\partial \overline{Z}}{\partial x_j} = \frac{\partial}{\partial x_j}\left[(D+D_T)\frac{\partial \overline{Z}}{\partial x_j}\right] \tag{4}$$

where $\overline{S}_{ij}$ is resolved strain rate tensor, ν and D are the kinemetic viscosity and molecular diffusivity.$\overline{Z}$ is the filtered mixture fraction. The mixture fraction is a normalized chemical element and is defined so that it takes the value of unity in fuel stream and zero in air stream. ν_T and D_T are the SGS turbulent viscosity and diffusivity, respectively. ν_T is calculated using the Smagorinsky model, with $\nu_T = C_s\Delta^2\left|\overline{S}\right|$and $D_T = \nu_T/\sigma_T$ [9]. σ_T denotes the turbulent Prandtl number.

2.1 Subgrid Scalar Treatment

Cook and Riley[11] proposed the beta distribution for the subgrid probability density function of the conserved scalar:

$$P(Z) = \frac{Z^{a-1}(1-Z)^{b-1}}{\int_0^1 Z^{a-1}(1-Z)^{b-1}\mathrm{d}Z} \tag{5}$$

Where

$$a \equiv \frac{Z}{\overline{Z'^2}}\left[Z(1-Z) - \overline{Z'^2}\right] \qquad and \qquad b \equiv \frac{1-Z}{Z}a$$

In equation (5) the function is parameterized by the filtered mixture fraction and subgrid scalar variance $\overline{Z'^2}$. The filtered mixture fraction is calculated using the scalar transport equation (eq.(4)). The variance term needs modeling. There are three common approaches used presently; a dynamic scalar variance model [12]; the scale similarity model [11] and; solving the evolution equation for variance[13]. Jimenez *et al* [13] have reported the superiority of the later method over the former two models. The SGS scalar dissipation rate appears in the evolution equation, and needs a model for closure.

The scalar variance is defined as :

$$g_z = \overline{Z'^2} = \overline{Z^2} - \overline{Z}^2 \tag{6}$$

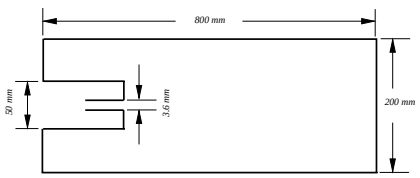

Figure 1: Geometric layout of bluff body burner

and its transport equation can be written as [13]

$$\begin{aligned}\frac{\partial(g_z)}{\partial(t)} + \frac{\partial \overline{u}_i \overline{g}_z}{\partial x_i} &= \frac{\partial}{\partial x_i}\left((D+D_T)\frac{\partial g_z}{\partial x_i}\right) \\ &- 2D\overline{\frac{\partial Z}{\partial x_i}\frac{\partial Z}{\partial x_i}} + 2(D+D_T)\frac{\partial \overline{Z}}{\partial x_i}\frac{\partial \overline{Z}}{\partial x_i}\end{aligned} \tag{7}$$

The filtered scalar Dissipation term $\overline{\chi} = -2D\overline{\frac{\partial Z}{\partial x_i}\frac{\partial Z}{\partial x_i}}$, can be modeled by assuming proportionality between the turbulent time scale τ and scalar mixing time scale τ_z [13]. The SGS scalar mixing time scale can be defined as:

$$\frac{1}{\overline{\tau_z}} = \frac{\overline{\chi}}{g_z} \tag{8}$$

Both time scales can be related such that:

$$\tau = C\tau_z \tag{9}$$

Where C is a model constant.

The turbulent time scale is the ratio of SGS kinetic energy and kinetic energy dissipation $\tau = \overline{\kappa}/\overline{\epsilon}$, and hence :

$$\overline{\chi} = C\frac{\overline{\epsilon}}{\overline{\kappa}}g_z \tag{10}$$

The value of parameter C is typically 2.0 [14]. A alternative value of C can be calculated by $C = 1/Sc$ [13], where Sc is the Schmidt number.

3 Simulation

A simulation has been performed of the bluff body flame experimental setup of Dally et al [15] using Star-CD Version 3.24. The setup comprises a 50 mm diameter bluff body and a fuel jet of 3.6 mm diameter. The overall size of domain is 800 mm in streamwise (X-axis), and

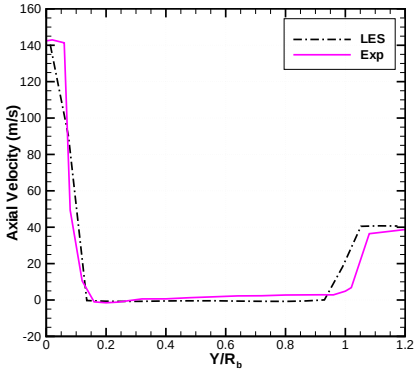

Figure 2: Axial velocity profile at $X/R_b = 0.2$

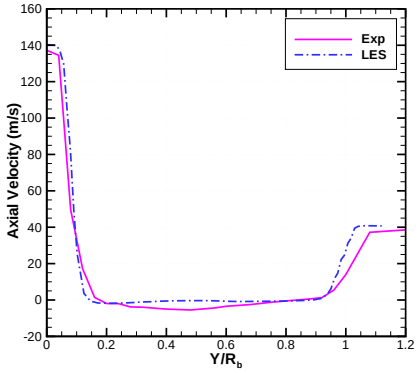

Figure 3: Axial velocity profile at $X/R_b = 0.54$.

200 mm in the spanwise(Z-axis) and the normal (Y-axis) direction(See Figure 1). An embedded mesh refinement technique has been used in and around the reacting zone. The areas of strongest shear have also been embedded with patches of fine mesh. A first order implicit scheme is used for temporal discretization, and the scalar transport equation for mixture fraction is solved using the MARS differencing scheme[16]. A central differencing scheme is used for the spatial discretization of momentum equation. Temperature, density and all chemical species are related to conserved scalar, the mixture fraction by [8]:

$$\overline{\phi} = \int_0^1 \phi(Z)P(Z)\mathrm{d}Z \tag{11}$$

where $P(Z)$ is given by eq. 5 and ϕ is any scalar. Two options are available in STAR-CD for the evaluation of equation (11).The first is to express the resulting functions as polynomials of the mixture fraction and perform the integration analytically. The second alternative is to employ a numerical integration technique. We have used the polynomial technique to express all scalars as a function of mixture fraction. The Prandtl and Schmidt numbers are assumed to be equal. The flow has low Mach number and a constant pressure is assumed in the domain. An adiabatic condition is assumed for the heat losses [17] from the domain. The inlet velocity for the coflow air is 40 m/s. The inlet velocities for the fuel jet are mapped from data derived from a separately simulated fully developed pipe flow. We have constructed the geometry so that the co-flow inlet boundary is 50 mm upstream of the bluff body exit plane. This ensures that velocity profiles are fully developed at the exit plane of the bluff body. Pressure boundary conditions are applied at all outer boundaries. The value of pressure is taken equal to atmospheric pressure i.e. 101325 Pa.

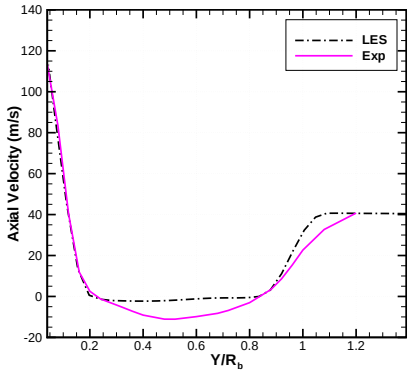

Figure 4: Axial velocity profile at $X/R_b = 1.2$.

4 Discussion

The averaged velocity profiles at different stations in the streamwise direction are plotted in comparison with the experimental data [15]. The comparison shows a good agreement up to an axial distance of approximately $X/R_b = 1.6$ down stream of the jet, where R_b refers to the radius of the Bluff body. The averaged velocities are plotted along the non-dimensional Y-axis(Y/R_b). Figures 2, 3 and 4 show the axial velocities at $X/R_b = 0.2, 0.54$ and 1.2 respectively. Velocities are overpredicted further down stream near the center line of jet. Figure 5 shows a comparison at $X/R_b = 1.8$, which reflects an overprediction in axial velocity at the centre line.

Muradoglu et al [18] have observed that a discrepancy exists in the experimental data at further down stream near the center line. In their simulation results they also found disagreement in velocities at downstream stations after $X/R_b = 1.6$, which was attributed to experimental errors. Dally et al [19] have also observed the same. This aspect still needs further investigation, to establish the actual reason for the disagreement. Mixture fractions plotted also show good agreement with the exper-

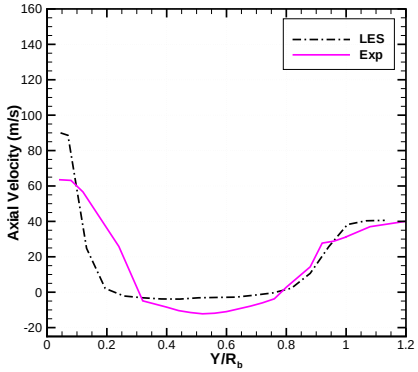

Figure 5: Axial velocity profile at $X/R_b = 1.8$.

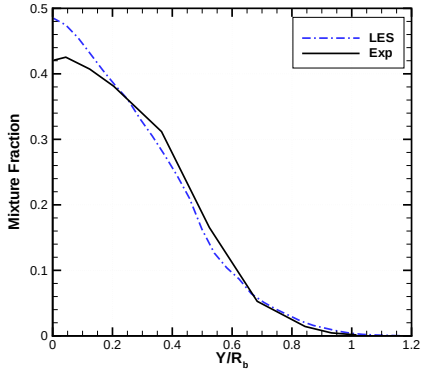

Figure 8: Plot of Mixture fraction at $X/R_b = 3.6$.

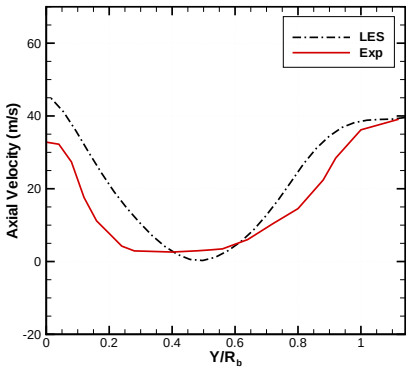

Figure 6: RAxial velocity profile at $X/R_b = 3.6$.

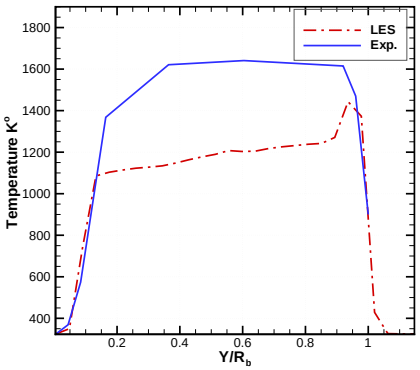

Figure 9: Plot of Temperature at $X/R_b = 0.6$.

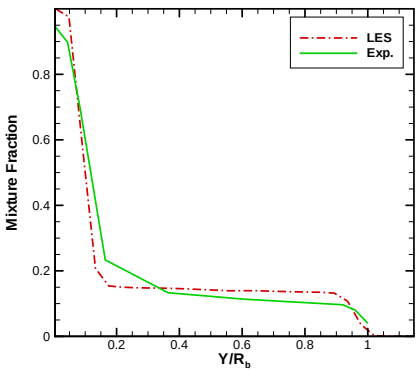

Figure 7: Plot of Mixture fraction at $X/R_b = 0.6$.

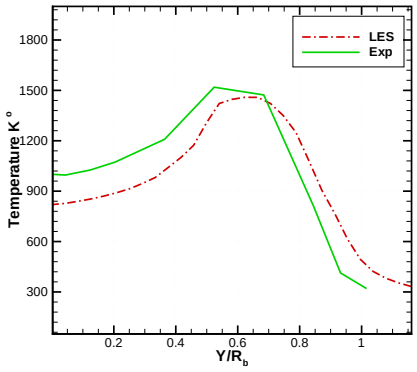

Figure 10: Plot of Temperature at $X/R_b = 3.6$.

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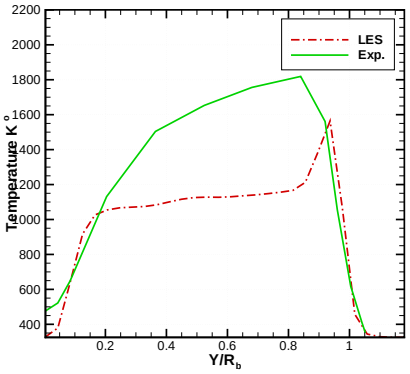

Figure 11: Plot of Temperature at $X/R_b = 1.2$.

imental data; Figures 7 and 8 show the comparison at $X/R_b = 0.6$ and 3.6, respectively. An over prediction of mixture fraction at the center line is also observed.The temperature profiles in Figures 9 and 11 do not show good agreement with the experimental data. The temperature is calculated via the PPDF, which itself is based upon the mixture fraction and its variance. The coefficient C used in equation 10 will affect the variance. An incorrect prediction of the variance will certainly affect the temperature. Dally et al [19] have observed the strong influence of model coefficient on mixture fraction variance. The temperature profile further down stream at $X/R_b = 3.6$ is not significantly distorted, this is may be due to mesh resolution. Because in the far field (i.e. $X/R_b > 3.0$), the effect of resolution is less important than in the inlet region. The low recirculation velocities (Figures 3, 4, 5) near the jet inlet also indicate a low mesh resolution.

5 Conclusions

A simulation of a bluff body burner using LES has been carried out. Our main focus was to demonstrate the application of the embedded mesh and the PPDF method for reacting flows. We have found reasonably good results for velocity profiles. The temperature profiles near the inlet and the recirculation velocities are underpredicted; this is due to the low mesh resolution.The temperature profile further downstream is acceptable. An optimised value of constant used for the scalar dissipation rate model is also needed for correct prediction of the reacting scalars. In our present study, our mesh size was limited to 3.5 million cells due to computational resources. A larger mesh of approximately 5.5 million cells is currently being studied. Further in our future work, we plan to study the effect of different SGS models and their coefficients on the prediction of mixture fraction variance and other scalars (i.e temperatures).

References

[1] S R Turns. *An Introduction to Combustion Concepts and Applications.* McGraw-Hill, Inc., 1996.

[2] U Piomeli. *Large-eddy and Direct simulation of Turbulent Flows (Lecture Notes).* Short course delivered at CFD2001 - 9 e confrence annuelle de la Socit canadienne de CFD. Kitchener, Ontario, 2001.

[3] U Piomelli, A Scotti, and E Balaras. *Large-eddy simulation of turbulent flows: from desktop to supercomputer (Invited Talk).* In Vector and Parallel Processing - VECPAR 2000. J.M.L.M. Palma, J. Dongarra and V. Hernndez (Springer:Berlin) , 2001.

[4] V Raman and H Pitsch. Large Eddy simulation of a bluff body-stabilized non-premixed flame using a recursive filter refinement procedure. *Combustion and Flame*, 142, 2005.

[5] C Wall, B J Boersma, and P Moin. An evaluation of the assumed beta probability density function subgrid-scale model for large eddy simulation of nonpremixed, turbulent combustion with heat release. *Physics of Fluids*, 12, 2000.

[6] P Givi. Model free simulation of turbulent reactive Flows. *Progress in Energy and Combustion Science*, 15, 1989.

[7] P J Colucci, FA. Jaberi, P. Givi, and S. B Pope. Filtered Density function for Large Eddy Simulation of turbulent reacting flows. *Physics of Fluids*, 10, 1998.

[8] A W Cook and J J Riley. A subgrid model for equilibrium chemistry in turbulent flows. *Physics of Fluids*, 6, 1994.

[9] S B Pope. *Turbulent Flows.* Cambridge University Press, 2000.

[10] S M deBruynKops and J J Riley. Mixing Models foe Large-Eddy Simulation of NonpremixedA Turbulent Combustion. *Fluids Engineering*, 123, 2001.

[11] A W Cook, J Riley, and P Givi. Model free simulation of turbulent reactive Flows. *Progress in Energy and Combustion Science*, 15, 1989.

[12] C. Jimenez, F. Ducros, B. Cuenot, and B. Bedat. A dynamic model for subgrid-scale variance and dissipation rate of a conserved scalar. *Physics of Fluids*, 10, 1998.

[13] C. Jimenez, F. Ducros, B. Cuenot, and B. Bedat. Subgridscale variance and dissipation of a scalar field in large eddy simulations. *Physics of Fluids*, 13, 2001.

[14] K N C Bray and N Peters. *in: P.A. Libby, F.A.Williams (Eds.)Turbulent Reacting Flows.* Academic Press, New York, 1994.

[15] B B Dally, A R Masri, R.S. Barlow, and G.J. Fietchner. Instantaneous and Mean Compositional Structure of Bluff-Body Stabilized Nonpremixed Flame. *Combustion and Flame*, 114, 1998.

[16] P N Asproulis. High resolution numerical predictions of hypersonic flows on unstructured meshes. *Ph.D Dissertation, Imperial College, Dept. of Aeronautics, London, England*, 1994.

[17] C H Priddin. *Turbulent combustion modelling a review. in: A V Johansson, P. h. Alfredsson (Eds), Advances in turbulence 3.* Springer-Verlag,Berlin/Heidelberg, 1991.

[18] M Muradoglu, K Liu, and S B Pope. PDF modeling of a bluff-body stabilized turbulent flame. *Combustion and Flame*, 132, 2003.

[19] B B Dally, D F Fletcher, and A R Masri. Flow and mixing fields of turbulent bluff-body jets and flames. *Combustion Theory Modelling*, 2, 1998.