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NO and CO formation in an industrial gas-turbine combustion chamber using LES with the Eulerian sub-grid PDF method

G. Bulat [a], W.P. Jones [b,*], A.J. Marquis [b]

[a] Siemens Industrial Turbomachinery Ltd., Waterside South, Lincoln LN5 7FD, UK
[b] Department of Mechanical Engineering, Imperial College London, Exhibition Road, London SW7 2AZ, UK

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ABSTRACT

The advances in computing power and numerical schemes allow Large Eddy Simulation (LES) to use more detailed turbulent combustion models as well as to be applied to real gas turbine combustors. In this work, we investigate the emissions formation in an industrial gas-turbine combustion chamber using LES with an Eulerian stochastic sub-grid pdf model with reduced chemistry. Sub-grid stresses are represented by a dynamic version of the Smagorinsky model and sub-grid species fluctuations are characterised by eight stochastic fields. The chemistry was represented by an ARM reduced GRI 3.0 mechanism with 15 reaction steps and 19 species. All calculations were carried out using a detailed block-structured mesh capturing all geometrical features of the Siemens SGT-100 burner operating at a pressure of 3 bar. The influence of the radiation heat losses was investigated and the impact of an alternative 4-step chemical mechanism was discussed. The results show good agreement with the experimental data. The NO formation rates were quantified with prompt NO dominating the thermal and N_2O formation paths.

1. Introduction

The challenge facing the industrial gas turbine for heat and power applications lies in meeting emissions regulations whilst running on a wider range of fuels, often with energy levels considerably lower than standard pipeline gas. Considering the importance of combustion and related issues, a reduction of emissions levels from gas turbine combustors is required. In addition to emissions requirements, the need to increase the life of component parts and their efficiency is paramount in reducing the cost of produced energy. For this challenge an in-depth understanding of physical processes is required, so that a more sustainable combustion process can be achieved.

The turbulent premixed flames found in industrial gas turbine combustors are difficult to study due to high levels of turbulence, fast chemistry and complex geometrical features. Most of these devices operate at high pressure, which adds to the difficulty of obtaining experimental data and accounting for pressure effects in computational simulation methods. Large Eddy Simulation (LES) is a powerful modelling technique particularly for highly swirling and unsteady flows. In the case of LES of turbulent combustion, account must be taken of the interactions between turbulence and the chemical reactions taking place. The main difficulties encountered in achieving this arise from the filtered chemical source terms, which represents the net rate of species formation through chemical reaction. Since heat releasing reactions are highly non-linear, the filtered values of the fields of chemical species mass fraction and temperature are strongly influenced by the sub-grid scale (sgs) fluctuations of the reactants and the temperature. One and perhaps the only method of accounting for these is through the introduction of the joint scalar probability density function (*pdf*) of all the relevant scalar quantities, which provides all the necessary information required to evaluate the filtered chemical source terms. LES has become very attractive for understanding the unsteady nature of complex flows, such as those in gas turbine combustors, [1]. The application of LES to gas turbine combustors is a subject of much current interest.

Several recent LES studies have been completed where comparisons with measured data have shown it capable of capturing different aspects of combustion. Extensive experimental data has been obtained in the Preccinsta experimental burner, [2,3], a Turbomeca radial burner operated at atmospheric conditions, resulting in *partially premixed* flames. Detailed LES for the reacting and isothermal cases have been completed. These include LES using a compressible unstructured solver in conjunction with an acoustic analysis, [4,5] where it was found that the PVC mode was very strong for the cold flow but disappeared with combustion taking place. The acoustic structure revealed by LES matches exactly the prediction of the acoustic solver for the 588 Hz mode. Excellent agreement was found between velocity fields arising from the LES and the LDV measurements. The above studies, however assumed

* Corresponding author.
E-mail address: w.jones@imperial.ac.uk (W.P. Jones).

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perfect mixing and some discrepancies between the LES results and experiments were identified. Subsequent studies on the same combustor, [6] have indicated that the level of premixing plays a significant role and cannot be ignored, especially for self-excited flame conditions. The fluctuations in equivalence ratio were shown to be associated with self-excited *combustion instability*. Moureau et al. [7] describe a detailed LES and DNS study of the Preccinsta combustor. A 2.6 billion cell mesh was used for the DNS study and the LES involved several mesh refinements with meshes with 1.7, 14, 110 and 329 million tetrahedral cells. The authors conclude the mesh resolution needs to be greater than one billion unstructured elements for the differences between the LES and DNS results to be negligible. However a relatively simple approach to turbulence-chemistry interactions was adopted with detailed laminar premixed flamelet results being tabulated in terms of two variables, mixture fraction and a reaction progress variable.

A more detailed LES study of the TECFLAM Burner, [8] has been completed with a flamelet approach, [9] and more recently with the *Eulerian stochastic field method*, [10]. It was demonstrated that the swirler geometry needed to be included to capture the complex swirling flame characteristics even in a relatively simple geometry, [9], in addition to a detailed representation of *sub-grid* chemistry, [10]. Other related studies include, for example, the LES of a swirl burner, [7] using a two parameter flamelet combustion model and the LES of combustion instabilities in a lean-partially premixed combustor, [6] using a two-step global mechanism. More detailed chemical reaction mechanisms have also been incorporated, for example in the LES of a non-premixed, temporally evolving, syngas/air flame using an 11-species, 21-step mechanism in conjunction with an artificial neural networks approach [11].

For combustion of liquid fuels, several LES studies of swirling flows have been performed in representative combustor geometries such as [12,1,13–15]. A recent LES study of atomisation on a radial burner MERCATO (which is very similar to the Preccinsta burner) was presented by [14] where mono-dispersed droplets were injected into a cross flow. It was found that both the gaseous and liquid predictions were in agreement with the experimental data. Again a PVC was identified and found to strongly influence the spray properties, defining droplet segregation, enhancing evaporation and generating droplet breakup.

In the context of LES and gas-turbine combustors the piloting effects on a Siemens gas turbine combustor using axial swirlers were studied, [16]. The dynamic thickened flame model was used in conjunction with a 2-step reaction mechanism, [17]. It was found that a PVC was present in the reacting case when a relatively small amount of pilot flow was present. It was demonstrated that the PVC captures some of the cold mixture gases (fuel and air) and inhibits their mixing with the surrounding products. The presence of the PVC in the reactive case was found to change the flame stabilisation point and to introduce instability of the precessing frequency. The injector characteristics of a GE LPP burner was studied [13]. where good agreement was found between the simulated results and measurements. LES has also been applied [18] to investigate the interactions of the flame and acoustics in the ALSTOM's EV burner. The main objective was to identify the effect of *combustion instability* and the heat transfer on NO_x emissions using the artificially thickened flame model. It was found that a more detailed representation of chemistry (beyond a 3-step mechanism) was needed.

All the above LES studies of industrial geometries involved simple chemistry (2 or 3-step), and the good agreement was generally obtained for the velocity fields often in conjunction with some over estimation of temperature and species concentrations. However, the use of simplified chemistry does not appear to allow the full potential of LES in capturing the turbulence and chemistry interaction to be exploited in complex geometries. The major objective of previous LES studies appears to have focused on capturing more turbulent features, rather than additional chemistry. On the other hand, relatively simple swirling flames have been well captured, [19], with detailed LES models accounting for interaction of turbulence and chemistry.

The studies reviewed above suggest a gap in the understanding of the complex nature of turbulent reacting flows in industrial geometries at high pressure conditions. The complexity of increased pressure on the reacting flow field presents a challenge for both computational and experimental studies. The flame thickness, δ_f is proportional to D/S_f and the time scale, τ_f is proportional to D/S_f^2 where D is the diffusivity and S_f is the laminar burning velocity. Since S_f is found to decrease slowly with pressure, p and D varies as p^{-1} the effect of increasing pressure is to reduce both the length and time scales of burning. As a result, the ratio of the turbulent time scale to the chemical time scale of the flow, defined as the *Damköhler* number, will increase as the pressure is increased and hence the flame regime may be affected. In addition, higher NO_x concentrations are likely to arise at high pressures. For this reason, the application of simulation methods with sufficiently detailed and accurate combustion models will almost certainly be required if flame behaviour in industrially relevant geometries is to be accurately reproduced. The *Eulerian stochastic fields* method in the LES framework presented in this work aims to provide an insight into the behaviour of such flames.

2. Mathematical model

2.1. Large Eddy Simulation

The LES-*pdf* formulation in conjunction with the Eulerian stochastic field solution method has been successfully applied in a range of burning configurations: ignition [20,21] and auto-ignition [22,23], non-premixed [24] and premixed regimes [19].

In LES the large scale energetic motions are computed directly with the effects of the unresolved sub-grid scale motions being modelled. The separation of the scales is achieved through a spatial filter, which for a function $f = f(\mathbf{x}, t)$ is defined as its convolution with a filter function G according to:

$$\overline{f}(\mathbf{x}, t) = \int_{\Omega} G(\mathbf{x} - \mathbf{x}'; \Delta(\mathbf{x})) f(\mathbf{x}', t) d\mathbf{x}' \tag{1}$$

The integration is defined over the entire flow domain Ω and the filter function has a characteristic width of Δ, which may vary with position. In the present work a 'box' filter defined by:

$$G(\mathbf{x} - \mathbf{x}'; \Delta(\mathbf{x})) = \frac{1}{\Delta^3}; \quad \mathbf{x}' - \Delta/2 \leqslant \mathbf{x} \leqslant \mathbf{x}' + \Delta/2$$
$$G(\mathbf{x} - \mathbf{x}'; \Delta(\mathbf{x})) = 0 \quad \text{otherwise}$$

is used.

In combusting flows large density fluctuations occur, which are incorporated through the introduction of density weighted (or Favre) filtered quantities, defined by $\tilde{f}(\mathbf{x}, t) = \overline{\rho f}/\overline{\rho}$. Applying the filtering operation, Eq. (1) to the conservation equations of mass and momentum leads to following set of filtered equations:

Continuity:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho} \tilde{u}_i}{\partial x_i} = 0, \tag{2}$$

Momentum:

$$\frac{\partial \overline{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \overline{\rho} \tilde{u}_i \tilde{u}_j}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\overline{\mu}\left[\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right]\right) - \frac{\partial}{\partial x_j}\tau_{ij} \tag{3}$$

where $\overline{\mu}$ is the filtered viscosity. The viscosities of the individual chemical species were determined from kinetic theory and the