MODELLING OF ION CHEMISTRY IN TURBULENT FLAMES FOR THE ANALYSIS OF NOVEL SENSORS FOR GAS TURBINE COMBUSTORS

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Abstract
The feasibility of using ion-current sensors to monitor the combustion process in a gas turbine is investigated by developing a numerical model able to predict the field of ionic species. Different kinetic schemes describing the formation and evolution of ions were preliminary tested in simple flames and then applied to the gas turbine combustor. Significant discrepancies were found between the available kinetic schemes in literature for the present conditions.

Introduction

The monitoring of combustion processes represents a central objective in combustion research, as fast and efficient diagnostics are needed to control and face events such as flame flashback or blowout.

Many efforts and advancements in this field have been made on internal combustion engines (ICEs) because of their great use in mobility. Waterfall et al. [1] provided an overview of the most important monitoring techniques used in ICEs underlining the use of ionization probes, optical fibres, laser methods and electrical capacitance tomography to detect the position and the dimension of the flame position, analysing also the sensitivity of the sensors to operating conditions such are the air to fuel ratio. Eriksson et al. [2] successfully used the spark plug in a sparked-ignited engine as an ion-current sensor. The spark was then employed as a pressure sensor for spark timing control, as the ionization current was observed to have a strong correlation with the cylinder pressure.

The application of these techniques to monitor combustion in gas turbines is more difficult because of the high temperatures, that can damage the sensors, and because of the geometrical complexity of the combustion chamber, that limits the possibility of inserting the sensors. However, one promising system is the Combustion Control And Diagnostics Sensor (CCADS) [3]. The CCADS is constituted by two electrodes, the sense electrode and the guard electrode. The first one, collocated near the air

inlet, can detect flashback, while the second one, placed close to the combustion chamber, allows the detection of the flame.
Wollgarten et al. [4] observed a close correlation between the ionization current signal and the chemiluminescence signal of OH*, that is often used to reveal the flame presence.
The present work is aimed at analysing the feasibility of the insertion of ion-current sensors to monitor the combustion process in a gas turbine. To this purpose, a numerical model of a simplified gas turbine is developed in order to get information on the distribution of the ionic species.

Methodology

Modeling ions in a gas turbine is a very complex problem, which involves several phenomena: turbulence, gas oxidation with formation and evolution of many radicals, formation of ions from some radicals and their evolution, and interaction of ions with the electric field which is applied at the electrodes of the sensor.
Here this complex problem was handled through a hierarchical validation procedure which is a common technique in CFD studies [5]. At the top of the hierarchy, reported in Figure 1 we found the main goal, which is the simulation of a gas turbine with an applied electric field, while at the lowest level of the pyramid we have the molecular processes and phenomena, which interact giving coupled problems. To address these phenomena, two benchmark cases were identified: a turbulent bluff-body flame and a laminar flame.
Three different kinetic schemes involving formation and evolution of ions were compared for the simulation of the bluff body flame, i.e. mechanisms of:

- Prager et al. [6], which includes 11 ions and 65 reactions, that were added to the GRIMech 3.0 w/o NO scheme for the chemistry of neutral species (35 species and 219 reactions).
- Rao et al. [7], containing 4 ions (i.e. HCO^+, H_3O^+, e^-, O_2^- [8]), 17 neutral species and a total of 22 reactions.
- Camara et al. [9], comprising 3 ions (i.e. HCO^+, H_3O^+, e^-), 29 neutral species (including 2 excited species, i.e. CH* and OH*) and a total of 73 reactions.

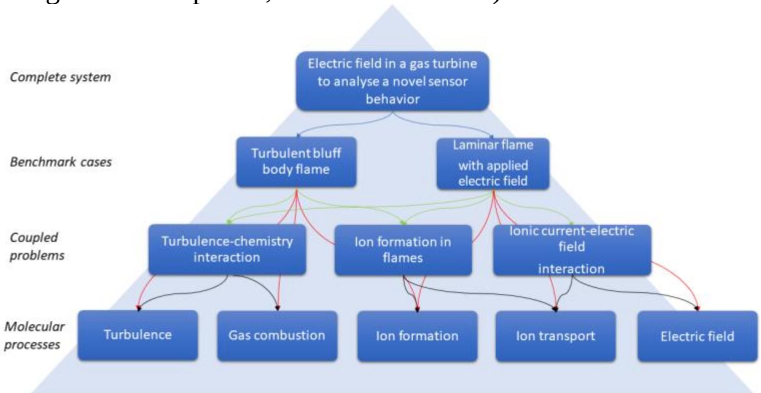

Figure 1 Hierarchical scheme for CFD study validation

An attempt was made to model the electric field and its effect on the transport of ions through the use of subroutines based on the local ion concentrations. However, simulations showed convergence problems, further stimulating the analysis of a simple laminar flame, not presented here.

Turbulent flame case and numerical model

The B1F1 bluff-body flame, experimentally characterized by the University of Sydney [10] (see Figure 3), was chosen because it is quite similar to the conditions in gas turbines environment. Methane is fed at a velocity of 67.0 m/s through a circular nozzle of ID=2 mm placed within two coaxial annular nozzles for the primary and the secondary air. Their injection velocities are 15.0 m/s and 2 m/s, respectively.

The numerical model was developed with ANSYS® Fluent 19.2. A 2D axisymmetric domain was used because of the symmetry of the system. The grid was structured with 42k cells and a grid convergence index GCI<3%.

Favre-averaged Navier-Stokes equations (FANS) were solved by closing Reynolds stresses with the realizable k-ε model and using the Eddy Dissipation Concept (EDC) as the model for interaction between turbulence and chemistry. Chemkin files were generated by merging the gas oxidation and ion chemistry. The thermodynamic and transport properties of the ions were taken as those for the neutral species.

Steady state simulations were run using a second order upwind interpolation.

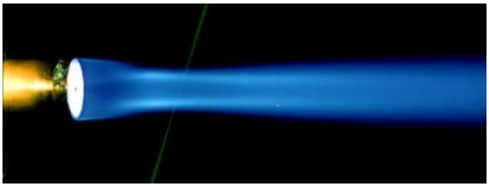

Figure 2 Image of B1F1 burner flame **[11]**

Gas turbine test rig and numerical model

The flame tube of the gas turbine combustor was modelled by using 1/8 of the geometry (see Figure 3) with periodic boundary conditions. A mixture of methane and air is supplied through the central nozzle by setting profiles of velocity, chemical species mass fractions and turbulence characteristics to take into account the presence of a swirled flow. The secondary air inlet is then collocated externally to improve the combustion process. The pilot, which feeds methane, is also shown in Figure 3. The grid was unstructured with 1.3M cells. The physical model was basically the same as for the bluff body flame, thus based on the solution of FANS equations with k-ε turbulence model and EDC combustion model, the latter coupled with mechanisms of Prager et al. [6] and Rao et al. [7].

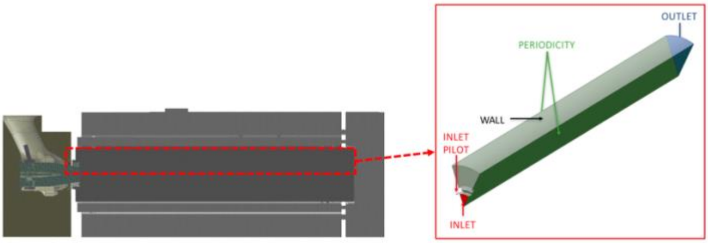

Figure 3 3D model of the gas turbine.

Results

The temperature distributions obtained for the B1F1 bluff-body flame with the three kinetic schemes are compared in Figure 4a and show a fairly good agreement. However, the axial profiles of temperature along the flame axis (Figure 4b) highlight some discrepancies; the trend is the same, but the mechanisms of Rao et al. [7] and Camara. [9] anticipate the flame quenching with respect to Prager et al. [6].

As for the ions, it was observed that the mechanism of Camara et al. [9] lead to much smaller concentration values (up to 3 orders of magnitudes) than that of Prager et al. [6]. Hence, Figure 5 compares only the mechanisms of Prager et al. [6] and of Rao et al. [7] for the prediction of radial profiles of e^- and H_3O^+, representing the most important ionic species, at axial distances x=40 mm and x=280 mm, corresponding to the initial and final region of the flame, respectively. The performance of the mechanism of Rao et al. [7] for the prediction of H_3O^+ may be considered satisfactory when compared the detailed mechanism of Prager et al. [6], especially considering the very small concentration values. However, e^- profiles indicate that e^- concentrations are strongly underestimated by Rao et al. [7].

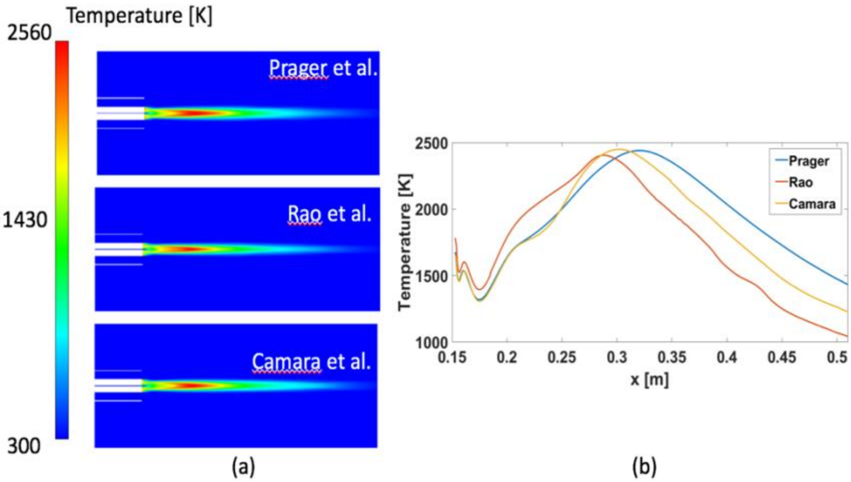

Figure 4 Temperature distributions (a) and profile along the axis of the bluff-body flame (b) predicted with mechanisms of Prager et al. [7], Rao et al. [8] and Camara et al. [11].

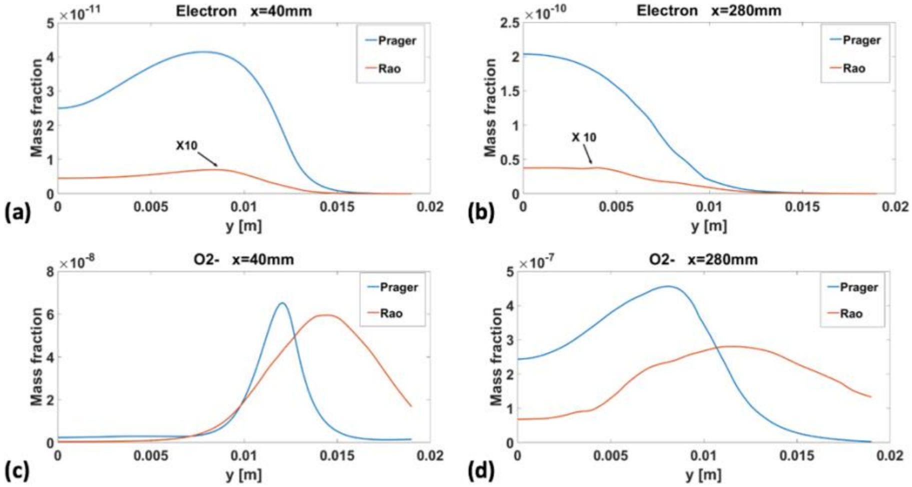

Figure 5 Radial profiles of e^- (a, b) and H_3O^+ (c, d) predicted with the mechanisms of Prager et al. [6] and of Rao et al. [7] at x=40 mm (a, c) and x=280 mm (b, d):

Similar comments hold also for the gas turbine combustor. The agreement between the mechanisms of Prager et al. [6] and of Rao et al. [7] for the prediction of the temperature field is satisfactory, however there are discrepancies on the concentration fields of e^- and H_3O^+. In particular the simulations with Rao et al. [7] indicates a strong accumulation of ions in the recirculation region above the pilot. This region however, is characterized by high temperatures so the insertion here of the ion-current sensor should be carefully checked.

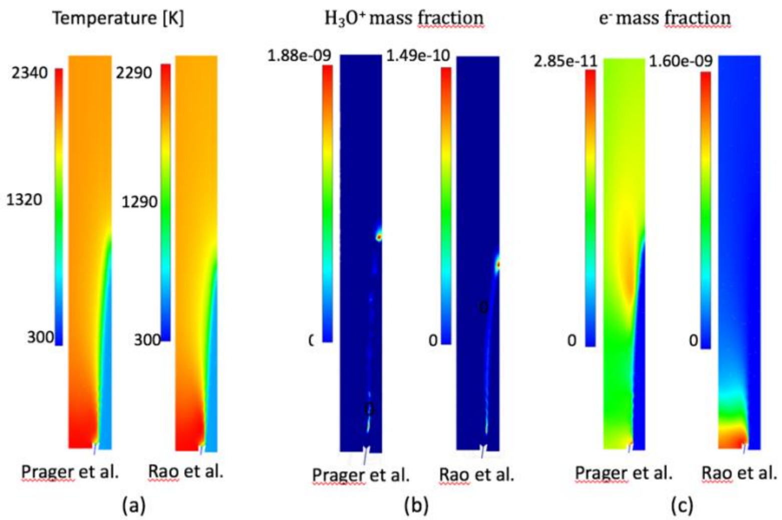

Figure 6 Distribution of temperature (a) and mass fraction of e^- (b) and H_3O^+ (c) predicted in the gas turbine with of Prager et al. [6] and of Rao et al. [7].

Conclusions

A CFD study of combustion, involving ion chemistry, in gas turbines had been done to investigate the possibility of the insertion of ion-current sensors. The use of reduced kinetic schemes leaded to significant differences especially in terms of the electron e^- concentration while better results were achieved for H_3O^+ when compared to the detailed mechanism of Prager et al. [6]. These findings were also confirmed on a bluff body flame.

Further efforts would be needed to include the presence of the weak electrical field imposed by an ion current sensor thus to analyze its effect on the transport of ionic species, even though the turbulent transport is probably dominating.

Acknowledgements

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