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**NUMERICAL SIMULATION OF WET COMBUSTION TO CONTROL NOX EMISSIONS
OF A HEAVY-DUTY GAS TURBINE COMBUSTOR**

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Abstract

Actually many gas turbines equipped with non-premixed combustion chamber are not able to operate, without hardware upgrades, due to the restrictions imposed by normative on NOx emission. The wet combustion could be an interesting way to control NOx with limited hardware modifications. Normally the setup of the wet combustion is performed with the support of very expensive and time-consuming experimental activities under full pressure operative conditions. On the contrary, numerical methods allow to study different configurations with limited resources. This paper presents a numerical investigation of the wet combustion in a heavy-duty gas turbine combustion chamber with particular attention to the reduction of NOx emission. The study is based on a simplified geometry derived from a real unit and the wet combustion is investigated by means of a discrete phase model for the management of water droplets. Results show that water injection influences heavily the temperature field and the NOx production. The study shows also how the droplet diameter is a key factor for the NOx emissions control.

Introduction

The current increase of the use of renewable non-programmable energy imposes the need of using gas turbines for the production during the daily power peaks. At the same

time, the present European regulation about NOx emissions introduces the necessity of upgrades on many machines but their cost is often too expensive compared with the machine value taken into account the expected operability. A possible way is the using of the wet combustion, it is based on the water injection within the combustion chamber to limit the temperature peaks so it permits to reduce the NOx formation from the Zeldovich mechanism [1].

Le Cong and Dagaut [2] show how the water flow rate influences the NOx production, showing a NOx reduction from 1000ppm to 80 ppm with only the 20% of water injected.

Dryer [3] in his work shows how the water influences the chemical kinetic in the flames thus to attribute the reduction of emission not only to the lower temperature but also to a different distribution of atomic oxygen and OH radical. This results are confirmed by Chen [4], he shows in detail how the water vapor reduces the concentration of atomic oxygen and the increasing of OH radical and this whets the reduction of NO. Other studies shows the increasing of the flame radical pool [5], [6] that support the thermal release and the promoting of micro explosions [7] those increase the fuel mixing.

The use of water gas turbines introduces complications about the potential increase of CO emissions and flame instabilities [8], these latter can cause mechanical stresses. The water must to be pure to ward off dangers to the combustors or the

turbine blades and also the operative conditions change because there is an increase of the mass flow rate in the turbine [9], [10]. Cardu et al. [11] analyses the thermodynamic cycles of a gas turbine with total water injection in combustion chamber and it reports the high level of thermal efficiency with a low level of NO_x emission.

Numerical simulations is powerful tool to understand some phenomenological aspects that are difficult to be investigated experimentally. Unfortunately only a limited amount of numerical investigations of wet combustion in gas turbine combustors are present in the scientific literature in fact the majority of works [12]-[14] are focused on the development of tools for the chemical kinetic influence of the water addition on some test-case flames.

Water addition isn't only a solution form heavy-duty gas turbine but it is proposed also for the turbojet engine, Benini et al. [15] carry out a numerical investigation to assess a combustion chamber, previously experimentally investigated. The its focus is the characterization of influence on NO_x emission caused by the increasing of water or steam flow, the NO_x reduction is assessed on 16% for the steam case and 8 % for the water case.

The more recently, Sun et al. [16] presents a work about the wet compression applied on a small turbojet engine. This work shows how the diameter of the water drops influences both the NO and CO emissions for the same water flow rate. Small droplets allow the reduction of NO emissions but CO emissions increase. The NO reduction promoted by small droplets dimension is mainly because water evaporates easily and this lead to enhanced reduction of the temperature peaks. The present paper concerns the numerical analysis of the wet combustion applied to a simplified geometry of heavy-duty gas turbine combustion chamber. The investigated case derives from an industrial

system fueled with natural gas and base on a non-premixed burner.

Nomenclature

CFD	Computational Fluid Dynamics
EDC	Eddy Dissipation Concept
MNS	Maximum Number of Steps
RANS	Reynolds-Averaged-Navier-Stokes
WFR	Water/Fuel Ratio

Numerical approach

1.1. Numerical models for turbulence, combustion and water injection

The aero-thermal phenomena that characterize a gas turbine combustor are in general very complex due to the interaction between chemistry and turbulence. These aspects are taken into account by the numerical approach, together with water injection which is managed by means of a discrete phase approach.

The CFD code used in this work is ANSYS Fluent® v14.5 [17]; its capability in modelling gas turbine combustion chambers was assessed in several previous analysis [18]-[20]. A steady RANS approach was selected for all the presented simulations. Concerning the turbulence closure Brewster et al. [21] and Hill et al. [22] suggest that the two-equation $k-\epsilon$ model is able to provide reasonable results for gas turbine combustion; based on this suggestion the realizable $k-\epsilon$ closure with standard wall functions for the near wall treatment was selected.

Combustion was modeled using EDC approach [23] combined with a simple two-step chemical mechanism for CH₄-air reaction. The choice of such approach was almost forced; in fact normally the use of the laminar flamelet concepts by Peters [24] with pre-processed chemistry allows the usage of more accurate chemical kinetics with limited computational costs. This model is not able to manage water injection because only two inlet streams (fuel and air) are

considered so the introduction of water through the dispersed phase would lead to an erroneous calculation of the local mixture fraction.

Since the NO_x concentration is very limited with respect to the other chemical species, it is reasonable to assume that NO_x generation does not affect the flow field, temperature and concentration of major combustion products. For this reason, the NO_x production was evaluated by means of a specific post-processing implemented in the code. The model used for NO estimation considers the pollutant produced via the thermal way (Zeldovich theory [1]) and through the intermediate N₂O [15]. Such approach was tested and validated on many works about gas turbine combustors [19], [25], [26]. As stated before, since the main objective of the work is to study water injection, a discrete phase approach was selected at this purpose. The model treats the gaseous phase as a continuum by solving the RANS equations while the injected water is treated like a dispersed phase by tracking a large number of droplets through the calculated aerothermal field. The discrete phase and the continuous phase interact reciprocally; the exchanges of momentum, mass, and energy of the dispersed phase with the continuum one are considered. The energy and mass transfers of the droplets are managed by a set of laws as a function of the droplet temperature: inert heating, vaporization and boiling. The so-called "inert heating" law acts when the droplet temperature (considered uniform on the droplet itself) is lower than the vaporization temperature; the solver computes an energy balance between each droplet and the surrounding fluid considering convective and radiative heat transfer. Heat and mass transfer are considered on the droplets due to vaporization and boiling when temperature reaches a critical temperature interval; the droplet temperature is updated

continuously based on sensible and latent heat.

1.2. Geometric model

The 3D model used as computational domain (Fig. 1) is a simplified geometry of an industrial can-annular combustion chamber. Due to the complexity of the original geometry only the fluid portion enclosed within the liner was taken into account, eliminating the outer casing and all the cooling holes along the liner. The swirler was not reproduced in the geometric model and an appropriate boundary condition was imposed.

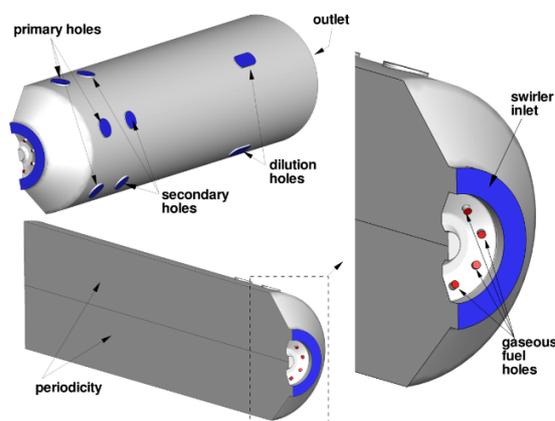


Fig. 1: Computational domain

The model has a 180° rotational periodicity with respect to the symmetry axis to permit a significant saving in computational costs. As it is possible to see from Fig. 1 a total amount of six inlet sections reproduces the primary and secondary air jets coming from the outer casing, while two elongated inlet sections reproduce the dilution holes.

1.3. Mesh

An hybrid unstructured mesh (Fig. 2) of the domain, composed by about 2.76M elements, was generated by means of the commercial code CentaurTM [27].

In order to adequately reproduce boundary layer, prismatic elements was added along the walls while the remaining part or the domain was filled by tetrahedrons. The height of the first prismatic cell along the walls was within the range of y^+ prescribed for the use of the near-wall treatment for the selected turbulence model.

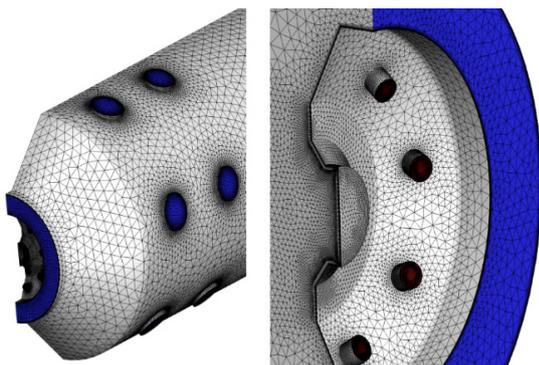


Fig. 2: Computational mesh; a detail of the burner is shown on the right

As visible in Fig. 2, particular grid refinements were enforced near the injection holes in order to adequately reproduce velocity gradients in those regions.

Water injection study

The first study that was conducted concerns water injection using a decoupled approach (the effects that water has on the main aero-thermal flow field are not considered). Simulations were performed in order to assess the conditions to be imposed for the discrete phase model in terms of: dimension of the droplets, injection velocity and wall condition. Both a cold flow case and a reactive case with an operating pressure of about 12.9bar were considered. For these studies, a uniform distribution of the particle diameter was imposed, while the mass flow rate of injected water has been fixed. Water is injected through the holes for the gaseous fuel indicated in Fig. 1.

Since no information about the dimension of the water particles was available, the effect of the droplet size on the evaporation process was initially investigated for the cold flow case. Three different particle diameters were considered: $1\mu\text{m}$, $10\mu\text{m}$ and $100\mu\text{m}$; for all the cases an injection velocity of 180m/s was imposed.

In order to assure the independence of the solution from the time step used for the integration of the droplet trajectories, three different values of step length factor were tested (1, 5 and 10). This latter parameter is defined as the ratio between the estimated transit time through a cell and the time step used for temporal integration. Negligible effects were observed from the sensitivity analysis on the step length factor and all the results shown in the follow are obtained with such parameter equal to five. The effects of the droplet size on the percentage of evaporated particles within the computational domain are reported in Fig. 3 as a function of the maximum number of time step (MNS) used to follow the trajectory of each single particle. As it is possible to observe the model predicts a very low evaporation rate for the $100\mu\text{m}$ case, even with high values of the MNS. The other two diameters of the droplets allow a complete evaporation of the injected water. A second test was performed using the hot flow case (results are not reported for brevity) observing that the discrete phase model is able to correctly reproduce the effect of the increased temperature in anticipating the evaporation.

Results shown in Fig. 3 were obtained with a reflecting condition for the droplets along the solid walls. In order to better understand what is the effect of the wall condition for the discrete phase model in determining the water evaporation, two additional simulations were performed considering other wall conditions referred as "trap" and "wall film".

For the first one, if the trajectory terminates on a wall, water instantaneously evaporates and the corresponding mass is added in the adjacent cell in the form of vapor.

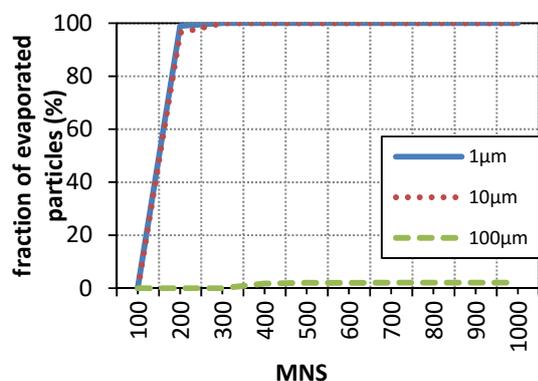


Fig. 3: Percentage of evaporated particles as a function of the maximum number of steps and the particle diameter (cold flow case)

For the second approach, the formation of a thin film is considered. The effect of the wall condition in determining the path length of the particles is reported in Fig. 4.

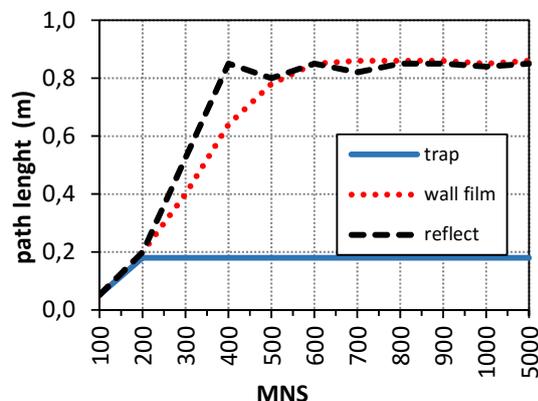


Fig. 4: Particle path length as a function of the maximum number of steps and the wall condition (hot flow case)

As it is possible to observe the trap boundary condition leads to the prediction of the shortest path because particles instantaneously evaporate after reaching a wall. In the other two cases a similar path length is predicted for high values of MNS.

After this study, the trap mechanism has been excluded for further simulations because of the very restrictive condition imposed, while the authors retained to be reasonable to proceed using the wall film condition that reproduces more physically the behavior of the droplets.

A further sensitivity study was performed about the injection velocity of the water droplets from the fuel holes.

Four different velocities were tested: 45, 90, 135 and 180 m/s. Results are shown in Fig. 5 in terms of residence time of the liquid particles.

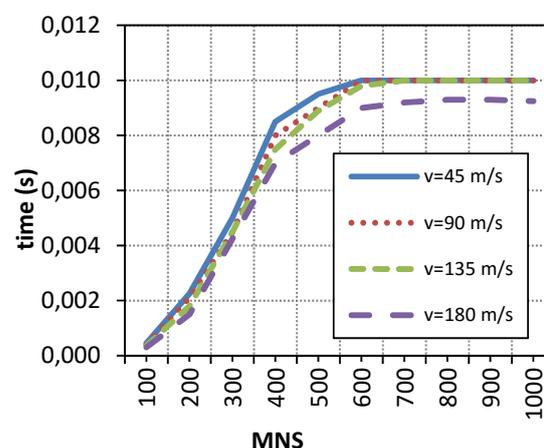


Fig. 5: Residence time of the particles as a function of the maximum number of steps and the injection velocity

As it is possible to see, for injection velocities lower or equal to 135 m/s the predicted residence time is almost independent from the initial velocity of the droplets. Considering the gas velocity though the fuel holes, which is about 180 m/s, it was retained reasonable to assume a lower injection velocity to take into account the inertia of the particles. For this reason, an injection velocity of 90 m/s was selected for the subsequent simulations.

Evaluation of temperature field and NOx reduction

After the sensitivity studies presented in the previous section, the assessed discrete phase model was used to evaluate the effect of water injection in terms of temperature fields and NOx emissions. Calculations are fully coupled, i.e. the interactions between continuous and discrete phase are considered. Two cases were evaluated, characterized by different water/fuel ratio (WFR). This parameter is the ratio between the mass-flow rates of injected water and fuel. The first case has WFR=0.5 while the second one is characterized by WFR=1. For both the test points two different diameters of the droplets were used: 10 μ m and 100 μ m. Results are reported in Fig. 6 in terms of temperature fields along a longitudinal plane passing through a fuel hole. In order to quantify the ability of water injection in reducing temperature, a comparison between dry and wet case is shown.

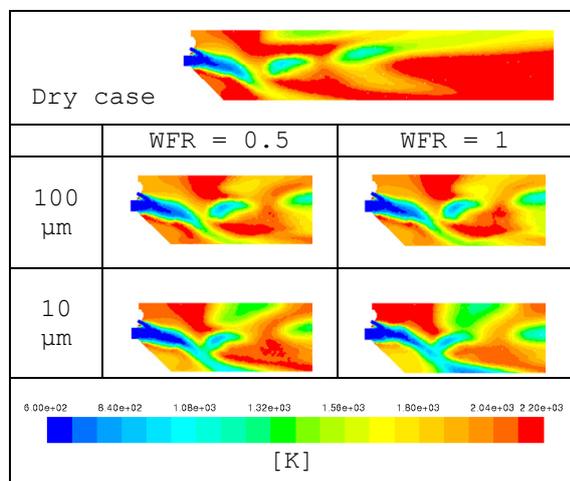


Fig. 6: Temperature [K] fields along a longitudinal plane passing through a fuel hole (dry and wet cases are shown)

As it is possible to observe, for the dry case, the high-temperature zones are more extended than in the wet cases. As expected, increasing the injected water mass-flow from WFR=0.5 to WFR=1, temperature reduction is

stronger, especially in the second half of the domain, where the dimension of the temperature peak over 2200K is drastically reduced injecting 100 μ m droplets and completely eliminated injecting 10 μ m droplets.

The effect of the reduction of the droplet size is beneficial for both the WFRs, but more pronounced with WFR=1.

As well known, the production rate of nitrogen oxides is strongly dependent from the presence of high-temperature peaks.

Consequently, the effect of water injection in reducing extension and intensity of high-temperature zones is beneficial from the point of view NOx emission reduction. This aspect was verified by means of a comparison between available experimental data and CFD results in terms of reduction of NO concentration at the discharge of the combustor (Fig. 7).

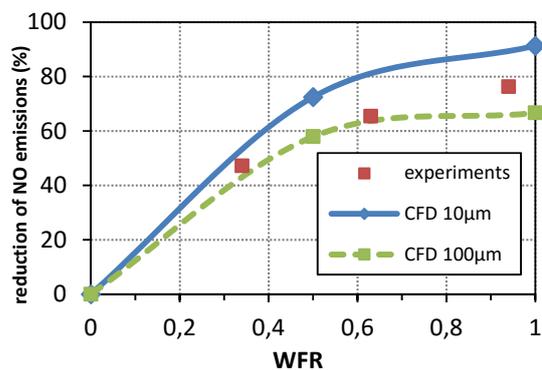


Fig. 7: Percentage reduction of NO emissions with respect to the dry case; comparison between CFD predictions and experimental data

It must be underlined that no information was available concerning the droplet dimensions of the experiments, consequently both the results obtained with 10 μ m and 100 μ m were used for the comparison. The reduction shown in Fig. 7 is referred to the reactive case without water injection.

As it is possible to observe the curves relative to the CFD simulations "contain" the experimental data, even if the 100 μ m

case is closer to the experiments with respect to the other one. As a general conclusion it is possible to state that the trend in predicting the reduction of emissions is correctly reproduced by the numerical simulations. In terms of concentration of NO at the discharge of the combustor, the effect of water injection is very strong, arriving till to a 74% abatement for a MFR of 94%.

Conclusions

A numerical method for the simulation of water injection into a heavy-duty gas turbine combustor with non-premixed flame was assessed and applied to the prediction of the reduction of NO_x emissions. In the initial phase the capability of the discrete phase model in evaluating the effects of different droplet sizes and injection velocities, as well as the condition to be applied along the solid walls for the management of the droplets, were evaluated by means of decoupled simulations. The discrete phase model was then applied to reactive cases, with different droplet sizes and WFR, considering the reciprocal interactions between continuous and discrete phase.

Water injection has shown to be very effective in reducing temperature peaks, especially in the second half of the combustor, leading to remarkable reductions of the NO emissions. Available experimental data in terms of reduction of NO concentration at the exhaust of the combustor was compared with the CFD predictions showing consistency in reproducing numerically the NO reduction as a function of the WFR.

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