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Modelling natural gas combustion in gas turbine: Coupling 3D combustion simulations with Chemical Reactor Network for advanced NOx prediction

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Gas turbine pollutant emissions (especially NOx and CO) are limited to 25 ppmvd by the European legislation for a natural gas operation. To meet this objective and the future legislations, it is crucial to have access to numerical tools that could predict quickly NO and CO emissions when operating gas turbine (fuel flexibility, tuning of the fuel distribution between burners…).
In this context EDF R&D has developed a 3D turbulent gas combustion model for several years. Nevertheless, the introduction of complex chemical kinetics in 3D turbulent combustion code is still too CPU time consuming to be performed for an industrial use. Thus, 3D CFD computations, using simple chemistry, are post-treated to generate a 0D Chemical Reactor Network (CRN), which includes a detailed chemistry mechanism. The 3D simulations are used to provide information about the mixing, and the aerodynamics including the turbulence effects.
The present study focuses on the impact of air ambient conditions (temperature and relative humidity) on NO production by industrial gas turbine. The detailed chemical kinetic scheme is at first validated on laboratory tests of jet-stirred reactor.

1. Introduction

To accurately predict minor species as NO and CO formations, it is necessary to couple Computational Fluid Dynamics (CFD) with a complex chemistry. Nevertheless, the introduction of detailed kinetics in 3D turbulent combustion code is still too CPU time consuming to be performed for an industrial use. Indeed, CFD solvers, optimized for the fluid dynamic but with restricted range of turbulence scales, could not be efficiently used to solve chemical equations for the full chemistry. Due to the stiffness of the underlying reaction scheme and the great number of species it contains, a partial coupling must be performed between CFD and detailed kinetics to save the computational demand.
This way of modelling keeps an accurate description of the kinetics. Most of the works performed with simplified flows are based on ideal chemical reactors. Initiated by Ehrhardt et al. (1998), these "hybrid" methods proposed a two-step procedure: firstly, fine grid CFD computations including global chemistry are used to calculate the

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turbulent flow in order to create afterwards a network of ideal chemical reactors based on a simplified flow model. Secondly, using a detailed chemistry, chemical reactors calculations are performed to determine precisely the production rate of minor species (NO, NO_2) and predict the total NOx emission.
In this work, the same way of modelling is carried on to generate a reactor network from Code_Saturne, the EDF CFD Code (freely available in open-source). The approach of chemical reactor network development is described by Fichet et al (2008).

2. Validation of chemical kinetic scheme

The chosen test case for validation is a jet-stirred reactor test facility used by Rutar (2000) and Rutar and Malte (2002) at the University of Washington. Measurements of NO and CO concentrations were performed in configurations close to the well stirred reactor combustion. It is a single burner injecting premixed air and natural gas mixture in an open small combustion chamber (1.5 cm3, see Figure 1) with ability for the test facility to operate under different pressure levels (up to 6.5 atm) and with different residence times of the gases in the combustion chamber. The mixture temperature as well as reactor temperature is measured with R-type thermocouples; equivalence ratio is controlled at the injection in order to maintain the reactor very close to isothermal combustion during NO and CO concentrations measurements (1815K at low residence time for all pressure levels and 1880K at long residence time for 4.7 and 6.5 atm and 1940K at long residence time for 3 atm case). This temperature control takes into account the heat loss of thermocouples which depends on residence time (mass flow rate and temperature).
The measurements were performed for a series of residence times from 0.5 to 4 ms and for three levels of pressure, 3, 4.7 and 6.5 atmospheres.

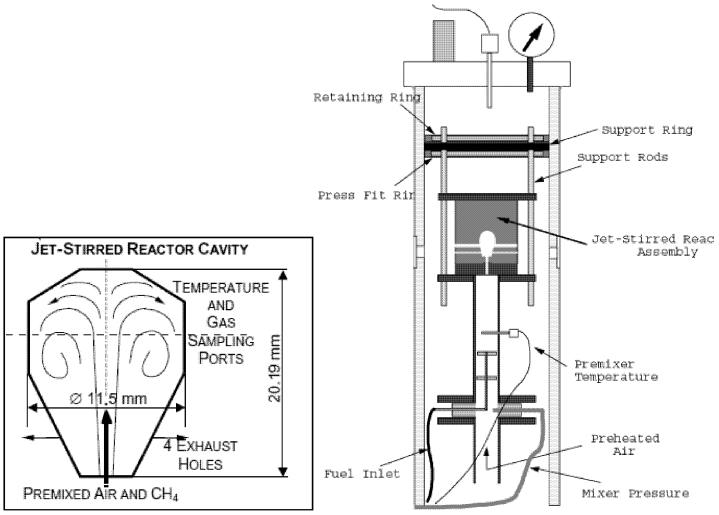

Figure 1: test facility of jet-stirred reactor (Rutar (2000) and Rutar and Malte (2002))

Rutar and Malte (2002) use Damköhler number (Da=characteristic time of turbulent mixing/characteristic time of chemical kinetic) and turbulence intensity to characterize the flame regime in the reactor. They show that, for the studied jet-stirred reactor, above the critical Da of 0.15, occurring when the residence time is above 2 ms, the reactor could be no more considered as perfectly stirred reactor. Thus, for cases where residence time is below 2 ms, the reactor is modeled using a single well stirred reactor module while two well stirred reactor modules are necessary for residence time above 2 ms.

Figure 2 shows the comparisons between the calculation and the measurements of Rutar and Malte (2002). The calculation results show the same trend as measurements: Starting at the lowest residence times, the NOx decrease with increasing residence time, reach a minimum, and then increase. The increase is caused by the increase in the combustion temperature for the largest residence times.

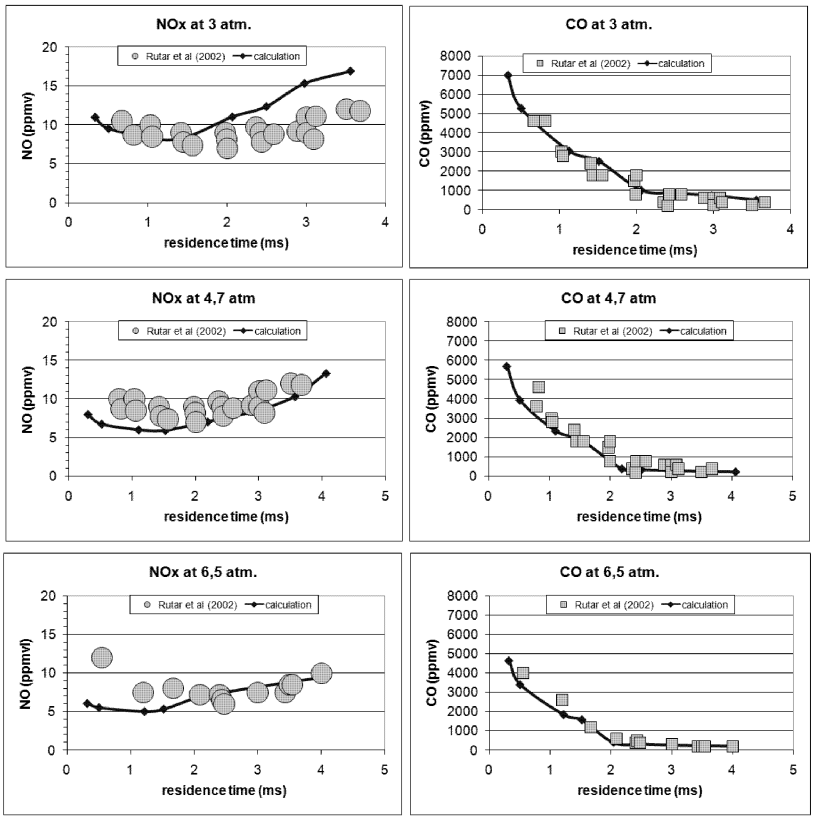

Figure 2: NO and CO concentrations (ppmv) versus residence time (ms) for different pressure levels (3, 4.7 and 6.5 atm) (line : calculation ; symbols : measurements (Rutar and malte 2002).

The NOx results for the 4.7 and 6.5 atm experiments can be compared in Figure 2 for the effect of pressure. For identical residence time, the experiments have nearly identical combustion temperature. Thus, the increase in NOx with decreasing pressure noted in Figure 2 is not masked by changing temperature. For the 3.0 atm experiments, the combustion temperature at residence times larger than 1.5 ms is greater than the temperature for the 4.7 and 6.5 atm experiments. Thus, the significant increase in NOx for the 3.0 atm data at the intermediate and large residence times is caused at least in part by the temperature increase (Rutar and Malte, 2002).

3. Application to industrial gas turbine

For industrial application a model of an industrial gas turbine operated by EDF is developed under the environment of the process simulator Aspen Plus™ (see Figure 3). The model iterates on the compressor pressure ratio while conserving the reduced flow rate of the turbine. The reduced flow rate, $\frac{Q.\sqrt{T}}{P}$, should remain constant for all operating parameters, where Q is the mass flow rate, T the temperature and P the pressure, all at the inlet of turbine. In order to simulate different ambient air conditions (temperature and relative humidity), characteristic curves of the gas turbine manufacturer, giving efficiency and flue gas mass flow rate versus ambient temperature, were used to evaluate the fuel and air mass flow rates of the gas turbine at different ambient temperature levels.

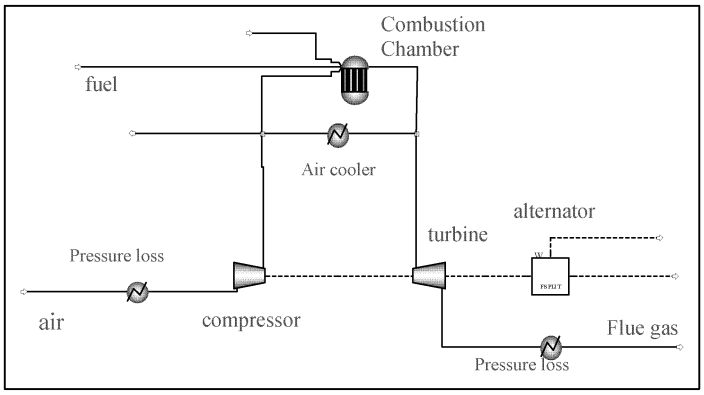

Figure3: process model of industrial gas turbine with Aspen plus™

3.1 Influence of ambient air temperature

This study encountered high difficulty in determining boundary conditions of the gas turbine because of few thermodynamic data is measured. The only measured mass flow rate concerns the fuel injection and its splitting among the different burners. Air mass flow rate is deduced from other measured parameters such as flue gas temperature and power plant electrical output. When nominal operating parameters are set up, the other operating parameters are determined using correlations deduced from the gas turbine

chart provided by gas turbine manufacturers. However, air splitting ratio concerning the combustion air and turbine cooling air and also splitting ratio of the air for premix burners and the air for non-premix burners are not measured. These parameters are for primary importance in NO prediction. This problem is solved by tuning the air combustion splitting in order to much NO value measured in the commissioning tests of the gas turbine. The air splitting ratio found with this calibration is then fixed for all other operating parameters. More accurate approach was developed by Fichet et al. (2008), a CFD was performed for air plenum simulating the air flow and its distribution between premix and non-premix burners. This computation gives also the velocity and turbulence profiles used as inlet data for combustion chamber modelling. Vincent et al (2008) includes also a scalar transport equation accounting for time live evolution of the fluid particles used as additional criteria for network reactor splitting; turbulence effect and residence time distribution in the reactors are also accounted for.

Figure 4 shows the variation of NO for different temperature levels (0-35°C) and at three levels of relative humidity, 0%, 60% and 100%. We can see that NO production decreases with increasing relative humidity whatever the level of temperature is. This figure shows also that under dried ambient air the NO production increases quickly with increasing temperature. For saturated air, the NO emission is almost constant and could even be lower at high ambient temperature than at lower temperature conditions.

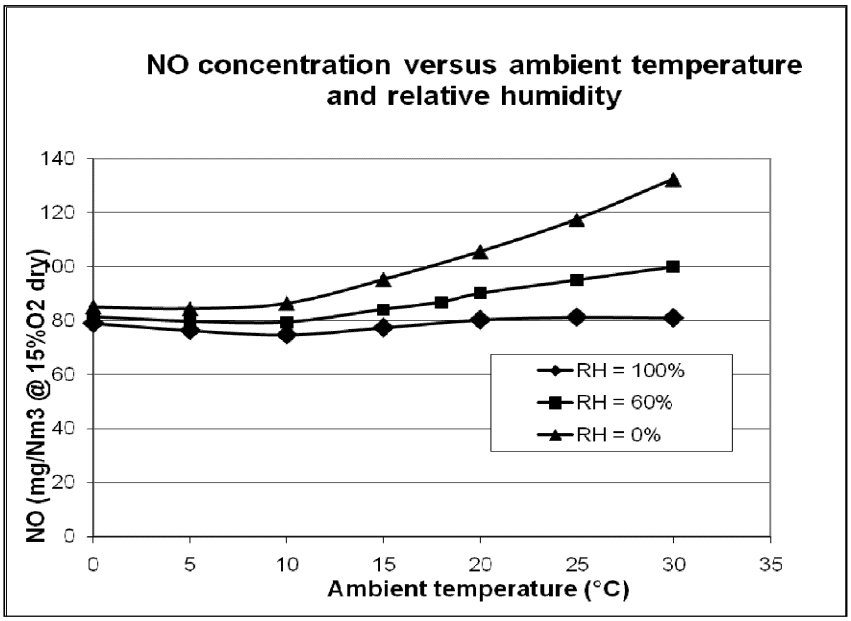

Figure 4: Influence of ambient temperature and relative humidity on NO emissions.

4. Conclusions

The work presented in this paper summarizes the development of numerical tool for NO prediction in industrial gas turbine using the approach of chemical reactor network. This approach uses CFD tool to build a network of reactors and to establish the flow rates of mass flow exchanged between the reactors. Full chemical scheme is then used in the reactor network to evaluate the temperature and concentration for more than fifty species including NO and CO.

Sensitivity analysis is given on the influence of ambient air temperature and relative humidity on NO emissions. This study evaluates how the NOx production increases with increasing temperature and how the relative humidity impacts this relation. NOx emission decrease with increasing relative humidity whatever the level of temperature is. Under dried ambient air, the NOx production increase quickly with increasing temperature. For saturated air, the NOx emission are almost constant and could be even lower at high ambient temperature than at lower ambient temperature.

5. Literature cited

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