MODELING GAS TURBINE COMBUSTION CHAMBER WITH THE CFX-5 AND CHEMKIN 3.7 PACKAGES

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Abstract. *The use of Computational Fluid Dynamics as a tool for designing combustion devices is, nowadays, of great importance. CFD codes, however, use simplified reactions mechanism for the combustion of hydrocarbon species. Conversely, the CHEMKIN 3.7 package calculates the fuel oxidation with detailed mechanism with major simplification for the reacting flow inside the combustor. The process of designing a combustor may be facilitated by the use of a network that combines well-stirred and plug flow reactors if there is a previous knowledge of the confined turbulent flow. The paper presents a methodology that can be used to optimize the design of the combustors using a CFD model and the CHEMKIN 3.7 package. Different combinations of networks were tested and the methodology is presented in this work. The main parameters studied were the length of the primary, secondary and dilution zone and emissions of NOx and other gases when propane is the fuel. The detailed mechanism employed was the Gri-mech 3.0, which has 53 species and 325 elementary reactions. The results have shown that by combining CFD simulation and the predictions from the a proposed network of simplified reactors, solved by the CHEMKIN package is n important tool to help designing gas turbine combustor.*

Keywords*. CFX-5, CHEMKIN 3.7, combustion, gas turbines, natural gas*

1. Introduction

The design of gas turbine combustor by means of numerical simulation is increasing substantially in substitution to a largely empirical development of the past. Gas turbine combustion chambers are responsible for the addition of energy directly to the flowing air in Brayton cycles. The fuels commonly used are natural gas, kerosene, Diesel, biogas among others. The physical and chemical phenomena observed inside the combustor are known to be very complex. The combustion chamber is the main source of pollutant emissions in such devices. Accurate predictions of the flow field as well as mixing characteristics and fuel conversion is a difficult task. Since tests facilities are becoming economically prohibitive, due to the inherent complexity of gas turbine combustors, there has been an increase in the utilization of designing tools, such as CFD codes. The introduction of a more theoretical approach had become necessary since conventional practices could not answer the new challenges imposed by more restrict environmental concerns, which claimed lower emissions and better overall performance.

Theoretical predictions are, historically, based on modular approach, in which the characteristics of the flow field was, to a certain extend, ignored, and by numerical simulation, mostly finite difference, of the three dimensional reacting flow. In the modular approach, the combustor is divided in different regions and modeled by partially stirred and plug flow reactors. In this type of solution, more complex reaction mechanisms can be used. As for the second approach, finite difference modeling, the flow field (conservation of momentum, mass, energy and chemical species) is more accurate solved but with simplified kinetics schemes. Each approach presents advantages and drawbacks.

Switbank et al (1979) presented a fundamental modeling of the main processes observed in gas turbine combustors, including the mixing, evaporation and kinetics in which a finite difference procedure for aerodynamic and thermal predictions was employed. Complementary stirred reactor algorithms were also used for estimating minor pollutant constituents. They claimed that experimental verification of the various predictions revealed remarkably good agreement between measured and predicted values.

In recent years, gas turbine combustors have been studied both, numerically and experimentally (Tolpadi et al., 1997; Cline et al., 1993; Gupta et al., 1991). In addition, detailed reaction mechanisms are increasingly more accurate and available for a broad range of fuels including those necessary for combustion-generated air pollution (Turns, 1996). Complex mechanism, though, are handled by very few numerical codes. The CHEMKIN 3.7 (Chou, 2002) package is a powerful software system for solving complex chemical kinetics problems. It has been widely used in predicting pollutant formation from different burning devices.

The CFX code has been used in predicting reactive flows in many combustion equipments. Jasbec et al. (2000) have used the CFX4 model to locate the ignition region for a lean methane mixture. For the computation of the main species conversion in the CFD code they derived a reduced kinetic mechanism that was tested against the detailed mechanism using the kinetic modeling software packages CHEMKIN II/SENKIN. Recently CFX code was employed in low-NOx combustor development (Zarzalis et al., 2002).

In this paper we present a solution procedure that complements the analysis of turbine combustors based on CFD modeling. More specifically, the combustor performance is first investigated by the CFX-5 code and the results are approximated and further analyzed by the CHEMKIN 3.7 package for the predictions of pollutant formation, based on a proposed network of well stirred and plug-flow reactors. This code version (CHEMKIN 3.7) is able to handle steady

and time-dependent properties of a well stirred reactor or a network of reactors through the AURORA routine. Such networks can include multiple inlet streams and recycling between reactor modules. The routine PLUG simulates a plug-flow type of reactor. These routines can, thus, be combined in order to simulate the entire gas turbine combustor with detailed kinetics mechanisms for the conversion of the fuel.

2. Solution Procedure

The geometry of the combustor (tubo-annular) was that proposed in the paper Jones and Toral (1983). Heitor and Whitelaw (1986) have characterized the flow in this type of combustor regarding velocity, temperature and species. Their study led to very important conclusions regarding the influence of combustion on the flow pattern compared to the estimated isothermal flow. This type of configuration was further studied by computational modeling in isothermal flow by Koutmos and McGuirk (1991). Figure (1) shows the gas turbine combustor geometry and its 3-D view.

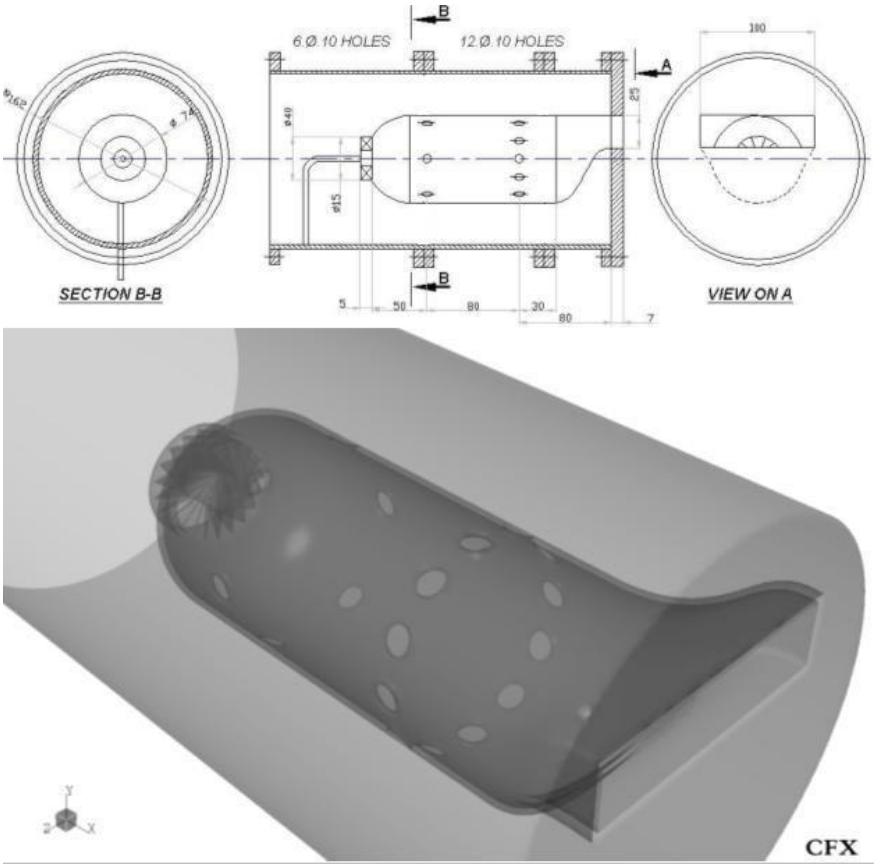

Figure 1: Model combustor geometry and 3-D view, adapted from Jones and Toral (1983).

The geometrical configuration proposed in Fig. (1) is of a single can combustor from a tubo-annular type of arrangement. As it can be seen, the combustor has swirl vanes for air injection into the flame tube and two rows of holes that characterize three different zones: (i) primary region responsible for anchoring the flame, between the swirler and the first row of holes, (ii) the secondary region, between the row of holes and (iii) the dilution zone, after the second row and before the exit. A summary of the CFX-5.1 command language for the predictions of the model combustor were as follows:

- Propane Air WD2, two steps global mechanism;
- Variable Composition Mixture;
- Species considered ⇨ C_3H_8,O_2,CO,CO_2,H_2O,N_2;
- Reference pressure ⇨ 1.0133×105 Pa;
- Simulation type was *Steady State*;
- Buoyancy model was *off*;
- Turbulence model was *k epsilon*;
- Turbulent wall functions were *Scalable*;
- Heat Transfer model was *Thermal Energy*;

- Combustion Model was *Eddy Dissipation*;
- Thermal radiation was *P 1* type;
- Inlet boundary condition for *air mass flow rate* was 0.0085 kg s^{-1};
- Inlet component *mass fraction* of oxygen was 0.232, nitrogen was constraint;
- Inlet *temperature* was 318 K;
- Inlet boundary condition for *fuel mass flow rate* was 0.00163 kg s^{-1};
- Inlet component *mass fraction* of C_3H_8 was 1.0;
- Inlet *temperature* was 318 K;
- Outlet boundary condition was *subsonic*;
- Wall boundary condition was *no slip*;
- Wall roughness was smooth;
- Wall heat transfer was adiabatic;
- Wall emissivity was 0.75

3. Results and Discussion

The parameters adopted here, for the code simulation, were the same of that presented in the paper of Heitor and Whitelaw (1986). We chose these values in order to check the CFX-5 against their experimental results. Our predictions are, at some extend, in good agreement to their measured values.

Figure 2 shows the streak lines through the model combustor. It can be seen the tangential velocity component after the swirler that helps to stabilize the flame. The flow is further perturbed by the two rows of holes before exiting the combustor. In Fig. (2) it is also possible to visualize the decaying of the swirling flow along the flow path. This plot, along with that for the temperature field were used for proposing the reactor's network for the analysis by the CHEMKIN package.

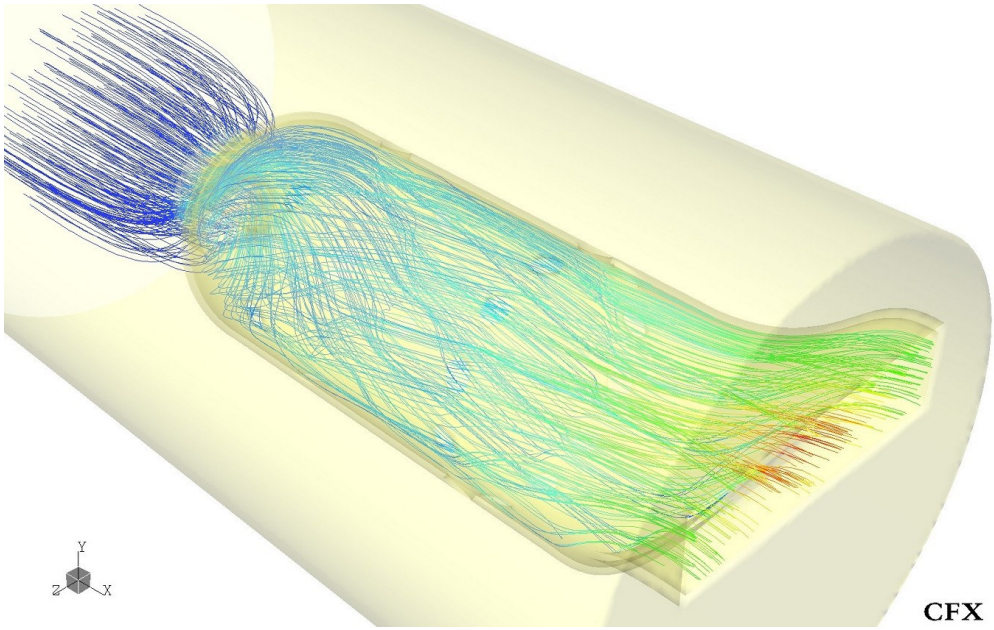

Figure 2: Streaklines in the proposed model combustor obtained by the CFX-5 code.

Figure (4) shows the predicted temperature field along the model combustor in the midaxial vertical plane. The predictions for this parameter are also in reasonable agreement to the experimental results of Heitor and Whitelaw (1986). For the average temperature at the exit of the combustor, we obtained 1151 K.

Following the analysis, a proposed network, based on the characteristics of the flow field, solved by the CFX-5 is shown in Fig. (4). The network was defined after exploring the aerodynamic behavior of the geometrical configuration of the gas turbine chamber and the operating conditions in terms of flow splits. The data regarding flow patterns can be taken from experimental measurements, numerical predictions or both. Therefore, reactor's volume and flow rates can be determined by integration of the velocity field at the limits of the proposed simplified reactor. As pointed by Turns (1996) useful results can only be achieved if the network designer has good previous experience. The technique adopted here is based on the work of Swithenbank et al. (1979), which applies the concepts of turbulent mixing to partially stirred reactors. The interconnected reactors may be changed to account for different flow patterns. The use of partially stirred reactors is possible due to the highly turbulent mixing in the primary region necessary to stabilize the flame, as

well as near the radial jets of dilution air. Stabilization of a flame is possible by anchoring it at some desired location where the local turbulent flame speed should match the local mean velocity (Turns, 1996) and self ignition is obtained by redirecting part of the hot combustion products to the primary zone as to heat the incoming fuel and air. Amid several methods the swirler was chose to provide the necessary recirculation zone.

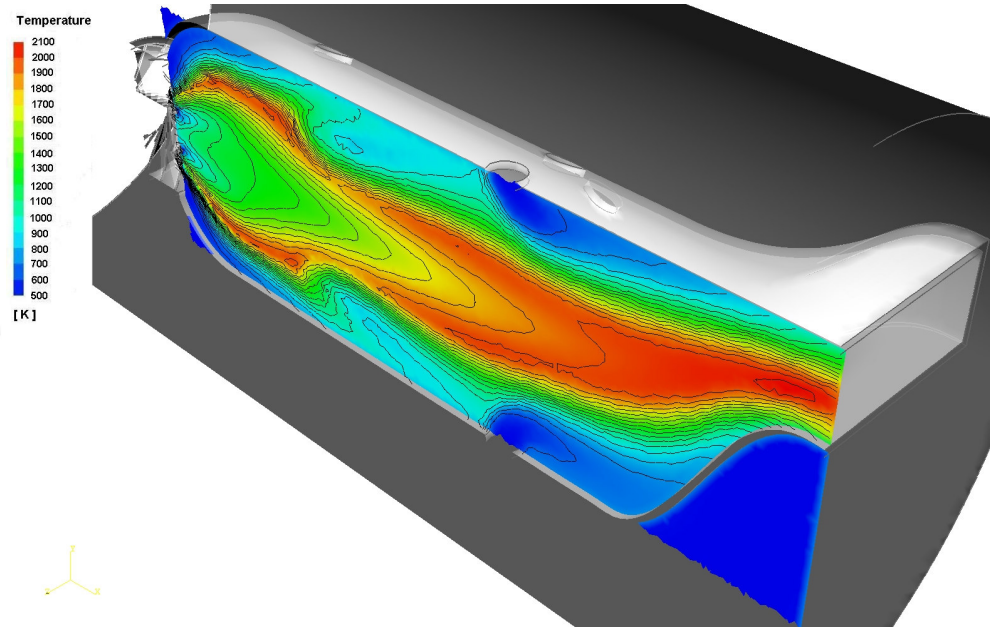

Figure 3: Temperature field in the model combustor, midaxial vertical plane.

In this work, we are primarily concerned to the introduction of such methodology with two advanced numerical tools, the CFX code and the last version of CHEMKIN package. The latter, as already mentioned, capable of handling reactor's network for steady or time-dependent problems. Therefore, the proposed network is not, and might be far from been, the best choice. The network consists of four reactors; three are of the type well stirred and the remaining is a plug-flow. Their relative location, size, ratio of mass to total mass and reactor's volume to the total combustor volume are described in the boxes. This network, as observed before, has the main purpose of presenting the methodology for such analysis. Increasing the number of reactors will certainly improve the quality of the investigation.

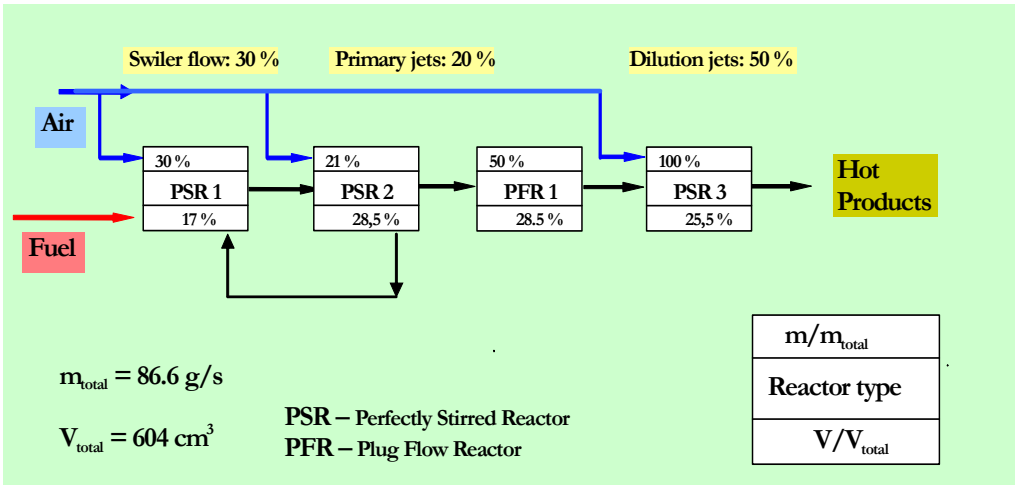

Figure 4: Proposed network for modeling the combustion chamber with the help of CHEMKIN 3.7 package.

To create the input data for the AURORA routine (perfectly stirred reactor – PSR) one must know the keyword syntax and the rules as to obtain useful results. Figure (5) presents a typical input data for a network of reactors showed as a summary in the output file of the AURORA routine. The parameters, such as the flow rate, gas composition (fuel

and air), temperature of the gases, pressure of the chamber (reactor) and, if it is the case, heat losses to the environments, reactor's volume and so on, must be provided. Since the AURORA routine handles network of reactors, recirculation and additional mass inlets may also be provided. Therefore, we choose the recirculation zone along with the region around the first row of holes to be solved directly by the routine. In Fig. (4) it corresponds to PSR 1 and PSR 2. The amount recirculation in the input data is such that the Keyword is RECY and the following numbers means from which reactor the flow comes and amount that is recycled. The amount of flow that recycles is obtained through integration of the flow field, in that desired location, from the predictions of the CFX-5 code. "RECY 2 1 0.15" means that 15% of the flow out of reactor 2 recycles to reactor 1. Reactor 2 (PSR 2) has one row of holes in its central volume flowing in the radial direction. This mass inlet is treated in the input file of the AURORA routine as "INLET primary air 2", meaning that air, as defined, is introduced in reactor 2. As it can be seen in Fig. (5), inlet streams are named for further control and distribution along the network.

The program is the allowed to run and the results, from this configuration, are used as an input data for the following plug-flow reactor. As regarded to the detailed mechanism, we used that proposed by Smith et al. (2003)

The output data from the AURORA routine presents the exit condition for each reactor in the network. For instance, temperature out of PSR 1 was 1977 K. The gas recycled from reactor 2 was at 1641 K. This investigation can also be extended for gas mole fractions. At the exit of the network, NO mole fraction is of 43.9 ppm, as calculated by the AURORA routine. As regarded to NO_x, the high temperature encountered at the exit of PSR1 indicates that the formation had its routes in the thermal mechanism. These finds are also in accordance with the experimental results of Heitor and Whitelaw (1986).

As mentioned, the data, at the exit of PSR 2 is the input parameter for PFR 1. The calculated residence time for this reaction and exit gas temperature were, respectively, 1.13 ms and 1692 K. As expected, the flow between the rows of primary and dilution holes extended the reaction. The output of PFR 1 was, then, used as input data for the last perfectly stirred reactor.

At the exit of the combustor, after PSR 3, the conditions are 1095 K and 22.3 ppm of NO. The average temperature predicted by the CFX-5 code was 1151 K. The global reaction mechanism, in the CFX-5 code, was absent of NO chemistry, therefore, no information could be obtained for nitrogen species other than N_2.

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        *               CHEMKIN Collection Release 3.7               *
        *                     AURORA Application                     *
        *              PERFECTLY STIRRED REACTOR MODEL               *
        * Copyright 1997-2002 Reaction Design.  All Rights Reserved. *
        ************************************************************

                WORKING SPACE REQUIREMENTS
                 PROVIDED        REQUIRED
 LOGICAL              196             196
 INTEGER            21707           21707
 REAL              337234          337234
 CHARACTER            174             174

Initializing CHEMKIN Gas-phase Library, a component of CHEMKIN Release
3.7. This and All Other CHEMKIN Libraries are Copyright (C) 1997-2002
Reaction Design.

          INLET STREAM FOUND FOR REACTOR     1: fuel
          INLET STREAM FOUND FOR REACTOR     1: primary air

KEYWORD INPUT
NPSR 2
ENRG
STST
TEMP 1500
PRES 1
QLOS 0.0
VOL 103.22 1
VOL 154.831 2
INLET fuel 1
INLET primary air 2
TINL fuel 318
TINL primary air 318
FUEL fuel C3H8    !"propane"
OXID fuel O2  0.23
OXID fuel N2  0.77
PROD fuel H2O
PROD fuel N2
PROD fuel CO2
EQUI 0.9296
REAC primary air O2   0.23
REAC primary air N2   0.77
FLRT fuel 26.638
FLRT primary air 18.2124
RECY 2 1 0.15
END
```

Figure 5: Input data for the AURORA routine for the first two reactors.

However, we were able to compare some major species, at the exit of the combustor, calculated by the CFD code and the proposed network in the CHEMKIN package. The discrepancies for O_2, CO_2, H_2O and N_2, were all less than 5%.

4. Conclusions

The application of the concept of turbulent mixing to partially stirred reactors is an interesting option to help in designing a gas-turbine combustion chamber. CFD analysis can be complemented with a modular network of reactors but using detailed mechanism for the reactions. Isothermal experiments and or numerical predictions might be enough to idealize a reactor's network that can be handled, cheaper and faster, by the CHEMKIN package. The analysis can be extended for the predictions of pollutant formation, mainly NOx, in gas turbine combustors as well as other combustion devices. In this paper we were able to estimate the emissions of NO starting from a CFD code run that had no kinetic rates for the conversion of nitrogen species.

5. Acknowledgement

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