A NUMERICAL STUDY OF CHEMICALLY REACTIVE FLOW OF HOT COMBUSTION GASES IN A FIRST-STAGE TURBINE NOZZLE

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ABSTRACT

Current progress in gas turbine performance is achieved mainly by increasing the turbine inlet temperature. At high temperature levels (>2000K), the hot combustion gases can no longer be considered as chemically inert, and it becomes important to account for dissociation and recombination reactions occurring not only in the combustion chamber but also within the expanding gas stream in the turbine. In this paper, the authors present a two-dimensional numerical study of chemically reactive flow of hot combustion gases through the first guide vane of a gas turbine. For this initial study, simplified boundary conditions are assumed: blade cooling air mixing is neglected, the blade wall temperature is assigned a fixed value, and uniform inlet conditions are assumed. This study investigates the effect of turbulence on chemical reaction kinetics and presents pollutant emission levels at the nozzle exit. Particular attention is also focussed on chemical reactivity near the pressure and suction sides of the turbine guide vane blades.

Greek Symbols:

\( \epsilon \) turbulent kinetic energy
\( \lambda \) thermal conductivity
\( \nu, \nu' \) stoichiometric coefficients
\( \rho \) density
\( \Phi \) equivalence ratio
\( \tau_{gg} \) stress tensor
\( \omega \) chemical species production rate

\( T \) temperature
\( u \) absolute gas velocity
\( z_i \) molar fraction
\( y_i \) mass fraction

Nomenclature

\( C_i \) concentration of species \( i \) in \( \text{mol m}^{-3} \)
\( k_f, k_r \) forward and reverse rate constants (units depend on reaction)

INTRODUCTION

In order to improve thermal efficiency, gas turbines have developed considerably in recent years with respect to their maximum working fluid temperatures and pressures. Ambitious research programs forecast gas turbine operation with Turbine Inlet Temperature (TIT) close to the stoichiometric flame temperature within the foreseeable future [2].

The analysis of the chemical behavior of the working fluid in gas turbines is usually restricted to the combustion chamber sections. However, at high temperature, the hot gases at the combustor exit do not only contain stable combustion products, but also contain dissociated species such as CO, OH, H2, etc. Thus, with the current trend towards high TIT, it is no longer correct to assume that the gases flowing through the hot section of the turbine are chemically inert. It is necessary to consider the recombination reactions of the dissociated species, resulting in heat release during the expansion.

Given the extremely fast changing aero-thermo-dynamical conditions during the expansion, the aforementioned chemical reactions are assumed to be far from equilibrium and, thus, governed by kinetics. A
coupled analysis with respect to both aerodynamics and thermo-chemistry becomes necessary when one aims to understand the impact of chemical reactivity on the flow characteristics in this part of the engine.

In a previous paper [3], the authors investigated the influence of chemical reactivity on the expansion characteristics in a stationary gas turbine using a one-dimensional flow model. A similar study was undertaken for the expansion characteristics in an aircraft turbo-jet engine [5]. These preliminary investigations showed clearly that at high turbine inlet temperatures, dissociated species are present at the turbine inlet. As the expansion proceeds, part of these dissociated species (mainly CO and H₂) recombine with oxygen, forming CO₂ and H₂O and releasing a further amount of heat. This heat release affects the expansion characteristics and is mainly observed in the first stage of the turbine. The study concluded that for hot combustion gas expansion in a turbine, chemical reactivity has a significant effect on the flow characteristics for nozzle inlet temperatures exceeding 2000 K.

Clearly, the conclusions that can be drawn from a one-dimensional model are limited, in particular because the chemical reaction rates are highly dependent on the fluid temperature, pressure and composition. In a 1-D model, these variables are assigned an average value for a given cross-section location within the flow region. In practice, however, the flow characteristics are such that this average value is not representative of local phenomena, in particular in the nozzle wall region. The purpose of this paper is therefore to present the results of a two-dimensional numerical study of chemically reactive flow of hot combustion gases in a gas turbine, using FLUENT CFD software. This study is restricted to the hottest part of the turbine where the phenomena described above are the most pronounced, i.e. the first guide vane. For this initial study, simplified boundary conditions are assumed: blade cooling air injection is neglected, the wall temperature is assigned a known value, and uniform inlet conditions are assumed.

DESCRIPTION OF THE 2-D FLOW MODEL

The main features of the proposed model are outlined below. The reader is referred to ref. [4] for a more complete description of the model.

Nozzle Geometry

The nozzle geometry considered in this study is that of Nuovo Pignone's PGT-10 model gas turbine, as described in ref. [8]. The blade characteristics are the following:

- axial chord: \( L = 53.401 \text{ mm} \);
- pitch at mid-span: \( 50.694 \text{ mm} \);

Fig. 1 shows the nozzle mesh grid. We note that the grid is refined close to the blades and in the throat section. The flow field considered includes an entrance section upstream of the nozzle guide vane.

Working Fluid Composition

In order to adopt realistic inlet conditions, it is necessary to perform detailed 2-D or 3-D simulation calculations of the combustor, which is beyond the scope of this study. Thus, uniform nozzle inlet conditions are assumed. As a result, important effects such as local fluctuations of the fuel/air ratio in the inlet flow stream are neglected. In order to compute the gas mixture composition at the combustor exit, we adopt the following hypotheses:

1. The gas mixture is free of hydrocarbon molecules;
2. Nitrogen oxides other than \( NO \) are only present in trace quantities, and can thus be neglected;
3. The mixture is assumed to be at chemical equilibrium, with the exception of the \( NO \) species;
4. The gas mixture contains the following 11 species: CO₂, CO, H₂O, H₂, OH, O₂, N₂, N and NO.

The combustor is modelled as a well-stirred reactor. Pressure drops and heat losses are neglected. The fuel (CH₄) is assumed to enter the combustor at the operating pressure and 300 K. The burnt-gas mixture composition at equilibrium at the combustor exit is easily computed for specified pressure and temperature (TIT) conditions using the STANJAN code [10]. The overall combustion equation can be written as follows:

\[
\Phi CH_4 + 2(O_2 + \frac{3.76}{1+0.16}N_2) \rightarrow 
\begin{align*}
 & n_1(z_{CO_2}CO_2 + z_{CO}CO + z_{H_2O}H_2O \\
 & + z_{OH}OH + z_{O_2}O_2 + z_{H_2}H_2 + z_{N2}N_2 \\
 & + z_{H}H + z_{N}N + z_{N2}N_2 + z_{NO}NO)
\end{align*}
\]

where \( \Phi \) denotes the equivalence ratio, and \( n_1 \) the total mole number \( n_1 = \frac{16.04}{3n_0 + 2z_{O_2} + z_{N2}} \). In practice, NO concentrations at the combustor outlet are considerably lower than those indicated by equilibrium calculations. Current Dry-Low-NOₓ type combustors can achieve NO emissions as low as 9 ppm running at full load on natural gas fuel. However, with higher TIT values, such low emission levels cannot be sustained. In this study, we set the NO mole fraction at the combustor outlet to 100 ppm. Clearly, this is an arbitrary choice. However, the NO concentration is well below the equilibrium value, and thus the production rate of NO is essentially independent of the initial concentration. If better estimations of the NO combustor outlet concentration are available, the results presented in this study can be easily corrected by introducing the appropriate offset.

**Flow Equations**

Real flow fields in turbomachinery applications present non-uniformities due to clearance effects, wake phenomena and secondary flows. Furthermore, unsteady pressure fluctuations, due to compressor operation and flame oscillations, occur in real operation at the expansion turbine intake. Since the intent of the present work is to provide basic information about the interaction between the working fluid chemical reactivity and its other flow characteristics, the current model is restricted to two-dimensional stationary flow phenomena. The model is further simplified by assuming adiabatic ideal gas flow.

The flow simulations were performed using the finite-volume CFD code FLUENT. The flow equations for chemical reactive flow implemented in this code are summarized below.

The conservation of species \( i \) is described by the following equation:

\[
\frac{\partial}{\partial x_a} (\rho u_a y_i) = -\frac{\partial}{\partial x_a} J_{i,a} + \omega_i
\]

where \( x_a \) denotes the spatial coordinate in the \( a \) direction, \( y_i \) is the mass fraction of species \( i \), \( J_{i,a} \) is the diffusive mass flux density of species \( i \) in the \( a \) direction and \( \omega_i \) is the net rate of production of species \( i \) per unit of volume due to chemical reactions. The summation of conservation equations for all the species present in the continuous phase results in the overall mass conservation equation.

Conservation of momentum in the \( a \) direction in an inertial reference frame is described as follows:

\[
\frac{\partial}{\partial x_a} (\rho u_a u_a) = -\frac{\partial p}{\partial x_a} + \frac{\partial \tau_{\alpha\beta}}{\partial x_a} + \rho g_a + F_a
\]

where \( p \) is the static pressure, \( \tau_{\alpha\beta} \) is the stress tensor and \( g_a \) and \( F_a \) are respectively gravitational acceleration and external body forces in the \( a \) direction. These two terms are neglected in this study.

Conservation of static enthalpy \( h \) yields:

\[
\frac{\partial}{\partial x_a} (\rho u_a h) = \frac{\partial}{\partial x_a} \left( \frac{1}{\rho} \frac{\partial T}{\partial x_a} \right) - \frac{\partial}{\partial x_a} \sum_i h_i J_{i,a}
\]

\[
+ u_a \frac{\partial p}{\partial x_a} + \tau_{\alpha\beta} \frac{\partial u_a}{\partial x_a} + S_h
\]

The source term \( S_h \) results from the heat released due to chemical reactions. The turbulence model used in this study is the standard \( k-\epsilon \) model.

**Chemical Reaction Kinetics**

The fluid undergoes rapidly changing temperature and pressure conditions while expanding through the turbine. To correctly account for the resulting fluid composition variations, a detailed chemical reaction mechanism scheme is considered (see ref. [3] for further details), as shown below:

**Reaction Mechanism**

<table>
<thead>
<tr>
<th>Reaction Mechanism</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 CO + OH \rightarrow CO₂ + H</td>
</tr>
<tr>
<td>2 CO + O + M \rightarrow CO₂ + M</td>
</tr>
<tr>
<td>3 O + OH \rightarrow O₂ + H</td>
</tr>
<tr>
<td>4 O + H₂ \rightarrow OH + H</td>
</tr>
<tr>
<td>5 H + H + M \rightarrow H₂ + M</td>
</tr>
<tr>
<td>6 H + O + M \rightarrow H₂O + M</td>
</tr>
<tr>
<td>7 O + O + M \rightarrow O₂ + M</td>
</tr>
<tr>
<td>8 N + NO \rightarrow O + N₂</td>
</tr>
<tr>
<td>9 N + O₂ \rightarrow NO + O</td>
</tr>
</tbody>
</table>
The production rate $\dot{\omega}_i$ of species $i$ that appears as a source term in Eq. 2 is computed as the sum of the production rates of species $i$ for the $j$ reactions in which the species participates:

$$\dot{\omega}_i = \sum_j \dot{\omega}_{i,j}$$

where $\dot{\omega}_{i,j}$ denotes the rate of production/destruction of species $i$ in reaction $j$. Reaction rate $\dot{\omega}_{i,j}$ is computed using an Arrhenius reaction rate expression, or by using the Magnusen-Hjertager eddy dissipation theory (see ref. [7]), depending on the turbulence intensity of the flow.

The Arrhenius rate is computed as follows:

$$\dot{\omega}_{i,j} = (\nu''_{i,j} - \nu'_{i,j})M_i \left[ k_{fj} \prod_i C_i^{\nu''_{i,j}} - k_{rj} \prod_i C_i^{\nu'_{i,j}} \right]$$

(5)

where $C_i$ is the molar concentration of species $i$, and $k_{fj}$ and $k_{rj}$ are the forward and reverse rate constants of reaction $j$. $k_{fj}$ is computed according to the standard Arrhenius formulation:

$$k_{fj} = A_j T_j^\beta_j \exp \left( - \frac{E_j}{RT_j} \right)$$

Data for the pre-exponential factor $A_j$, the temperature exponent $\beta_j$ and the activation energy $E_j$ are taken from ref. [9]. The reverse rate constants $k_{rj}$ are related to the forward rate constants through the reaction equilibrium constants.

As mentioned above, the influence of turbulence on the reaction rate is taken into account by using the Magnusen-Hjertager eddy dissipation theory [7]. In this model, the reaction rate $\dot{\omega}_{i,j}$ is given by the smallest (i.e. limiting) value of the two expressions below:

$$\dot{\omega}_{i,j} = (\nu''_{i,j} - \nu'_{i,j})M_i \frac{y_{i,R}}{k_{fj} M_R}$$

(6)

$$\dot{\omega}_{i,j} = (\nu''_{i,j} - \nu'_{i,j})M_i B P \frac{y_{i,P}}{\sum_P y_{i,P} M_P}$$

(7)

where:

- $y_{i,P}$ represents the mass fraction of any product species $P$;
- $y_{i,R}$ represents the mass fraction of a particular reactant $R$ which gives the smallest value of $\dot{\omega}_{i,j}$;
- $A$ et $B$ are two empirical constants equal to 4.0 and 2.0 respectively.

The eddy break-up model relates the rate of reaction to the rate of dissipation of the reactant and product containing eddies. $k/\epsilon$ represents the time scale of the turbulent eddies according to the eddy break-up model of Spalding. In turbulent reacting flows, the code calculates the reaction rates from the Arrhenius expression (Eq. 5) and the eddy break-up model (Eqs. 5 and 7). The limiting (slowest) rate is used as the reaction rate and the contribution to the source terms in the species conservation and enthalpy equations are calculated from this reaction rate. Heat released by the chemical reactions is accounted for in the source term of the enthalpy equation and is defined as follows:

$$S_h = \sum_i h_i^s \dot{\omega}_i$$

Since the NO production rate is considerably slower than that of the other chemical species, the Magnussen theory can no longer be considered. In this study, the NO production rate was thus computed using only the Arrhenius reaction rate.

The reaction rates are computed using the CHEMKIN-II package [6] coupled to the CFD code.

Wall Boundary Conditions

The first stage nozzle of a high temperature turbine is generally equipped with a sophisticated blade cooling system to maintain acceptable blade temperature levels. Complete simulation of such a complex system is beyond the scope of this study. We recall that cooling air mixing is neglected in this study. Thus, the nozzle wall boundary conditions considered are blade wall temperature profiles. Figure 2 shows the surface temperature profiles of a film-cooled turbine blade, based on numerical and experimental results obtained by Arnone et al. [1]. Based on these results, a simplified blade wall temperature profile is imposed for the simulation calculations, as shown in Fig. 3. The first case considered ($T_w1 = 1100$ K, $T_w2 = 800$ K) is representative of current turbine technology. The second case ($T_w1 = 1560$ K, $T_w2 = 1080$ K) is representative of future high performance blade materials and cooling systems.

Simulation Conditions

The purpose of this study is to provide basic information on the interaction between chemical reactivity and flow field characteristics at high temperature. Preliminary results obtained using a 1-D model (see refs. [3] and [5]) showed that such effects are most significant for operating conditions close to stoichiometric. Thus, in this study, simulations were run for only one turbine inlet temperature and operating pressure: TIT=2400 K and p=40 bar.
As we discussed previously, the gas mixture leaving the combustion chamber is assumed to be completely free of hydrocarbon molecules and to also be at equilibrium. Uniform inlet conditions are assumed at the $i = 1$ plane, as listed in Table 1. $l_i$ and $I_i$ represent turbulence length and turbulence intensity respectively. The values retained for this study are taken from ref. [8].

Table 1: Nozzle inlet conditions

<table>
<thead>
<tr>
<th>$P_0$</th>
<th>40 bar</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_0$</td>
<td>2400 K</td>
</tr>
<tr>
<td>$\equiv CO_2$</td>
<td>$7.7844 \times 10^{-2}$</td>
</tr>
<tr>
<td>$\equiv CO$</td>
<td>$1.3213 \times 10^{-3}$</td>
</tr>
<tr>
<td>$\equiv H_2O$</td>
<td>$1.8547 \times 10^{-1}$</td>
</tr>
<tr>
<td>$\equiv O_2$</td>
<td>$3.5395 \times 10^{-2}$</td>
</tr>
<tr>
<td>$\equiv H_2$</td>
<td>$4.6573 \times 10^{-4}$</td>
</tr>
<tr>
<td>$\equiv OH$</td>
<td>$3.3091 \times 10^{-3}$</td>
</tr>
<tr>
<td>$\equiv O$</td>
<td>$2.4883 \times 10^{-4}$</td>
</tr>
<tr>
<td>$\equiv H$</td>
<td>$5.2221 \times 10^{-5}$</td>
</tr>
<tr>
<td>$\equiv N$</td>
<td>$2.4976 \times 10^{-8}$</td>
</tr>
<tr>
<td>$\equiv NO$</td>
<td>$1.0000 \times 10^{-4}$</td>
</tr>
<tr>
<td>$\equiv N_2$</td>
<td>$7.2616 \times 10^{-1}$</td>
</tr>
<tr>
<td>$l_i$</td>
<td>0.075 m</td>
</tr>
<tr>
<td>$I_i$</td>
<td>3 %</td>
</tr>
</tbody>
</table>

RESULTS

Effects of Turbulence and Pollutant Emissions

In order to emphasize the influence of turbulence on reaction rates, simulations were performed:

- using only Arrhenius reaction rates;
- using the limiting reaction rate (i.e. the slowest of the rates computed using Arrhenius and Magnussen theory).

Table 2 presents average values of pressure, temperature and mole fractions at the nozzle exit. We observe significant differences between the two simulation cases, particularly for CO, $H_2$, and all atomic species. As the gas expands, the reaction rates computed by Magnussen theory become lower than those computed by Arrhenius theory, leading to a net decrease of recombination reaction rates, and resulting in higher exit concentrations for these species.

Fig 4 shows the CO mole fraction profile along the central plane $j = 18$. During the expansion process, the rapid decrease of temperature and pressure favors the recombination of CO to form CO$_2$. However, this process is governed by reaction kinetics and the exit CO concentration twice the equilibrium value ($x_{CO,eq} = 5.4 \times 10^{-4}$). Furthermore, we note that the outlet CO mole fraction computed assuming Magnussen
Table 2: Nozzle exit compositions for different reaction rate assumptions

<table>
<thead>
<tr>
<th>Component</th>
<th>Arrhenius rate</th>
<th>Arr. &amp; Mag. rate</th>
<th>Δ%</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{CO_2}$</td>
<td>1.03</td>
<td>0.76</td>
<td>32</td>
</tr>
<tr>
<td>$P_{CO}$</td>
<td>2.84</td>
<td>2.48</td>
<td>14</td>
</tr>
<tr>
<td>$P_{H_2}$</td>
<td>3.56</td>
<td>3.28</td>
<td>9</td>
</tr>
<tr>
<td>$P_{H_2O}$</td>
<td>2.35</td>
<td>2.09</td>
<td>11</td>
</tr>
<tr>
<td>$P_{N_2}$</td>
<td>7.26</td>
<td>7.26</td>
<td>0</td>
</tr>
</tbody>
</table>

Reactivity Near Nozzle Walls

In this study, we also investigated the effect of nozzle wall temperature on chemical reaction rates. Two simulations of reactive flow were performed with different nozzle wall temperature profiles, as discussed previously. In this section we present NO, CO and $\Delta T$ profiles for the following three axial locations:

- nozzle inlet (plane $i = 25$);
- midway section (plane $i = 60$);
- nozzle outlet ($i = 90$).

Fig. 6 shows the NO mole fraction profiles. We note first of all that the nozzle wall temperature level has little effect on the NO production. At the nozzle inlet, we note a slight increase of NO production close to the nozzle walls due to the increased gas residence time in the leading edge region. The profiles obtained for the two other locations show that NO production is higher in the pressure side region of the flow. This can be explained by a less pronounced temperature decrease along the pressure side compared to the suction side. We note a difference of more than 150 ppm between the two zones. This effect is further illustrated in Fig. 7, which shows NO mole fraction contours in the flow field.

Fig. 8 shows CO mole fraction profiles. We again note the reduced effect of nozzle wall temperature levels. We further note that the three profiles are very similar, with the following characteristics:

Figure 4: CO mole fraction profile along $j = 18$ plane

Figure 5: $\Delta T$ along $j = 18$ plane
- in the core of the gas stream, the production rate of CO is essentially constant;
- close to the walls, we observe a net decrease of CO mole fraction due to the low gas temperature, which shifts the equilibrium of reactions 1 and 2 (see Reaction Mechanism).

Fig. 9 presents CO mole fraction profiles throughout the nozzle.

As discussed previously, this recombination of CO to CO$_2$ releases a considerable amount of heat. Fig. 10 presents $\Delta T$ profiles for three $x$ locations and two blade wall temperature distributions. We again note the
small influence of the nozzle wall temperature level. The figure shows that the heat released by recombination of dissociated species results in an increase of temperature near the walls, which could cause a reduction of blade cooling performance. However, further study is necessary in order to draw conclusions regarding the impact of chemical reactivity on blade cooling performance. In particular, this study neglects cooling air injection, which will affect the chemically reactive flow around the blades considerably, due to an increased oxygen concentration near the blade surface, and a lower temperature in the wall boundary layer region.

CONCLUSIONS

The results presented in this paper show that the dissociation/recombination reactions occurring in the first guide vane of the turbine have a significant impact on the flow characteristics in this section of the engine. Thus for future high TIT gas turbines, it will become necessary to account for chemical reactivity of the combustion gases in order to correctly estimate performance and environmental characteristics.

A key result of this study is that turbulence tends to considerably reduce the rate of recombination reactions, resulting in increased CO pollutant emission levels. Another key result is that heat is released due to the recombination of CO, which modifies the gas stream characteristics during the expansion process. This is mainly observed close to the blade walls which may impact on blade cooling performance. However, further study is necessary before drawing conclusions on this topic.

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References


