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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 (> 2000 K), 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.

T	temperature	K
u	absolute gas velocity	$m\ s^{-1}$
x_i	molar fraction	$mol_i\ mol^{-1}$
y_i	mass fraction	$kg_i\ kg^{-1}$

Greek Symbols:

ϵ	turbulent kinetic energy dissipation rate	$m^2\ s^{-3}$
λ	thermal conductivity	$W\ m^{-1}\ K^{-1}$
ν', ν''	stoichiometric coefficients	–
ρ	density	$kg\ m^{-3}$
Φ	equivalence ratio	–
$\tau_{\alpha\beta}$	stress tensor	$N\ m^{-2}$
ω_i	chemical species production rate	$kg_i\ m^{-3}\ s^{-1}$

Nomenclature

C_i	concentration of species i	$mol\ m^{-3}$
k_f, k_r	forward and reverse rate constants (units depend on reaction)	
F	external body forces	$N\ m^{-3}$
g	gravitational constant	$m\ s^{-2}$
h	specific mass enthalpy	$J\ kg^{-1}$
h_f^0	mass formation enthalpy	$J\ kg^{-1}$
i	x direction grid coordinate	–
j	y direction grid coordinate	–
J_i	diffusive mass flux density	$kg_i\ m^{-2}\ s^{-1}$
k	turbulent kinetic energy	$m^2\ s^{-2}$
L	blade chord	m
M	molar mass	$kg\ mol^{-1}$
n_t	total mole number	mol
p	pressure	Pa
R	molar gas constant	$J\ mol^{-1}\ K^{-1}$
S_h	chemical heat source term	$W\ m^{-3}$

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, H_2 , 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-thermodynamical conditions during the expansion, the above-mentioned 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 H_2) recombine with oxygen, forming CO_2 and H_2O 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 practise 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:

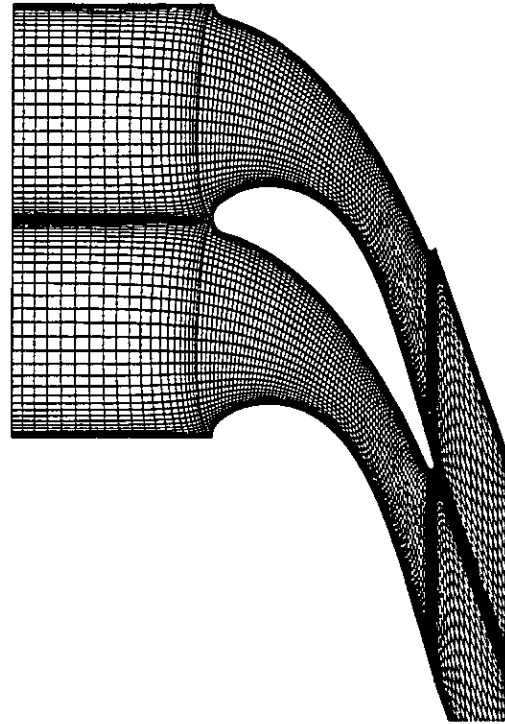


Figure 1: Geometry and mesh ($ixj = 121 \times 36$ grid) of the first guide vane

- axial chord : $L = 53.401$ mm;
- pitch at mid-span : 50.694 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.

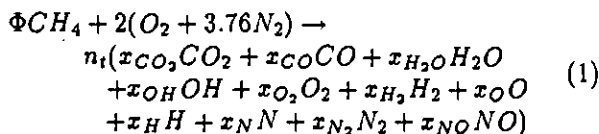
Working Fluid Composition

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:
 $CO_2, CO, H_2O, H_2, H, OH, O_2, O, N_2, N$ and NO .

The combustor is modelled as a *well-stirred reactor*. Pressure drops and heat losses are neglected. The fuel (CH_4) 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:



where Φ denotes the equivalence ratio, and n_i the total mole number $n_i = \frac{15.04}{2x_{N_2} + x_{NO} + x_N}$. In practice, NO concentrations at the combustor outlet are considerably lower than those indicated by equilibrium calculations. Current Dry-Low-NO_x type combustors can achieve NO_x 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:

$$\frac{\partial}{\partial x_\alpha}(\rho u_\alpha y_i) = -\frac{\partial}{\partial x_\alpha} J_{i,\alpha} + \dot{\omega}_i \quad (2)$$

where x_α denotes the spatial coordinate in the α direction, y_i is the mass fraction of species i , $J_{i,\alpha}$ is the diffusive mass flux density of species i in the α direction and $\dot{\omega}_i$ 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 α direction in an inertial reference frame is described as follows:

$$\frac{\partial}{\partial x_\beta}(\rho u_\alpha u_\beta) = -\frac{\partial p}{\partial x_\alpha} + \frac{\partial \tau_{\alpha\beta}}{\partial x_\beta} + \rho g_\alpha + F_\alpha \quad (3)$$

where p is the static pressure, $\tau_{\alpha\beta}$ is the stress tensor and g_α and F_α are respectively gravitational acceleration and external body forces in the α direction. These two terms are neglected in this study.

Conservation of static enthalpy h yields:

$$\frac{\partial}{\partial x_\alpha}(\rho u_\alpha h) = \frac{\partial}{\partial x_\alpha} \left(\lambda \frac{\partial T}{\partial x_\alpha} \right) - \frac{\partial}{\partial x_\alpha} \sum_i h_i J_{i,\alpha} + u_\alpha \frac{\partial p}{\partial x_\alpha} + \tau_{\alpha\beta} \frac{\partial u_\alpha}{\partial x_\beta} + S_h \quad (4)$$

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	
1	$CO + OH \rightleftharpoons CO_2 + H$
2	$CO + O + M \rightleftharpoons CO_2 + M$
3	$O + OH \rightleftharpoons O_2 + H$
4	$O + H_2 \rightleftharpoons OH + H$
5	$H + H + M \rightleftharpoons H_2 + M$
6	$H + OH + M \rightleftharpoons H_2O + M$
7	$O + O + M \rightleftharpoons O_2 + M$
8	$N + NO \rightleftharpoons O + N_2$
9	$N + O_2 \rightleftharpoons NO + O$

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 Magnussen-Hjertager *eddy dissipation* theory (see ref. [7]), depending on the turbulence intensity of the flow.

The Arrhenius rate is computed as follows:

$$\dot{\omega}_{i,j} = (\nu''_{i,j} - \nu'_{i,j})M_i \left[k_{f,j} \prod_i C_i^{\nu'_{i,j}} - k_{r,j} \prod_i C_i^{\nu''_{i,j}} \right] \quad (5)$$

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

$$k_{f,j} = A_j T^{\beta_j} \exp \frac{-E_j}{RT}$$

Data for the pre-exponential factor A_j , the temperature exponent β_j and the activation energy E_j are taken from ref. [9]. The reverse rate constants $k_{r,j}$ 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 Magnussen-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 :

$$\dot{\omega}_{i,j} = (\nu''_{i,j} - \nu'_{i,j})M_i A \rho \frac{\epsilon}{k} \frac{y_{i,R}}{\nu'_{i,R} M_R} \quad (6)$$

$$\dot{\omega}_{i,j} = (\nu''_{i,j} - \nu'_{i,j})M_i B \rho \frac{\epsilon}{k} \frac{\sum_P y_{i,P}}{\sum_P \nu''_{i,P} M_P} \quad (7)$$

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/ϵ 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. 6 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:

$$S_h = \sum_i h_{f,i}^o \dot{\omega}_i$$

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.

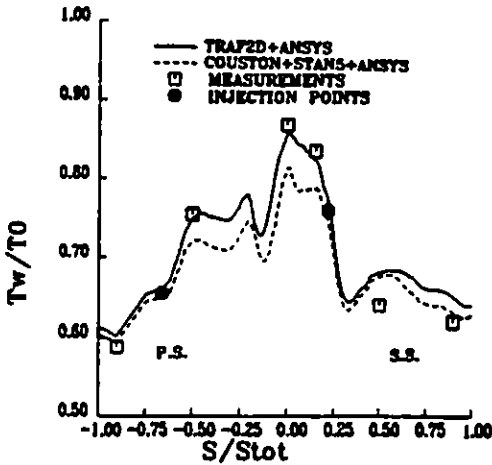


Figure 2: Blade temperature profiles from Ref.[1]

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_t and I_t represent turbulence length and turbulence intensity respectively. The values retained for this study are taken from ref. [8].

P_{03}	40	bar
T_{03}	2400	K
x_{CO_2}	7.7484	$\times 10^{-2}$
x_{CO}	1.3213	$\times 10^{-3}$
x_{H_2O}	1.5547	$\times 10^{-1}$
x_{O_2}	3.5395	$\times 10^{-2}$
x_{H_2}	4.5573	$\times 10^{-4}$
x_{OH}	3.3091	$\times 10^{-3}$
x_O	2.4883	$\times 10^{-4}$
x_H	5.2221	$\times 10^{-5}$
x_N	2.4976	$\times 10^{-6}$
x_{NO}	1.0000	$\times 10^{-4}$
x_{N_2}	7.2616	$\times 10^{-1}$
l_t	0.025	m
I_t	3	%

Table 1: Nozzle inlet conditions

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 ($x_{CO,eq} = 5.4e-4$). Furthermore, we note that the outlet CO mole fraction computed assuming Magnussen

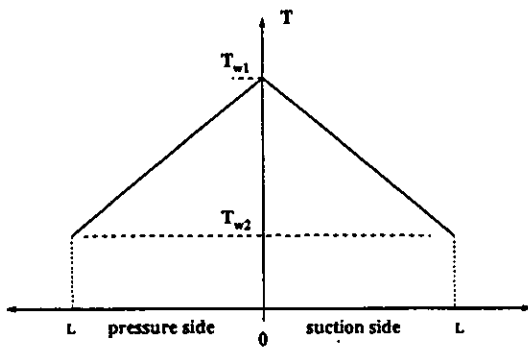


Figure 3: Blade temperature profile: T_{w1} = leading edge temperature, T_{w2} = trailing edge temperature

		Arrhenius rate	Arr. & Mag. rate	Δ %
p	(bar)	27.14	27.14	0
T	(K)	2215	2211	0.2
x_{CO_2}	$\times 10^{-2}$	7.86	7.86	0
x_{CO}	$\times 10^{-3}$	0.70	1.03	32
x_{H_2O}	$\times 10^{-1}$	1.56	1.56	0
x_{O_2}	$\times 10^{-2}$	3.50	3.51	0.2
x_{H_2}	$\times 10^{-4}$	3.19	3.81	16.3
x_{OH}	$\times 10^{-3}$	2.35	2.45	4
x_O	$\times 10^{-4}$	1.35	1.98	31.8
x_H	$\times 10^{-5}$	2.66	4.08	34.8
x_N	$\times 10^{-9}$	4.38	6.25	30
x_{NO}	$\times 10^{-4}$	6.76	6.83	1
x_{N_2}	$\times 10^{-1}$	7.26	7.26	0

Table 2: Nozzle exit compositions for different reaction rate assumptions

theory is well above that computed using Arrhenius reaction rates. Consequently, we observe a large amount of CO at the nozzle exit.

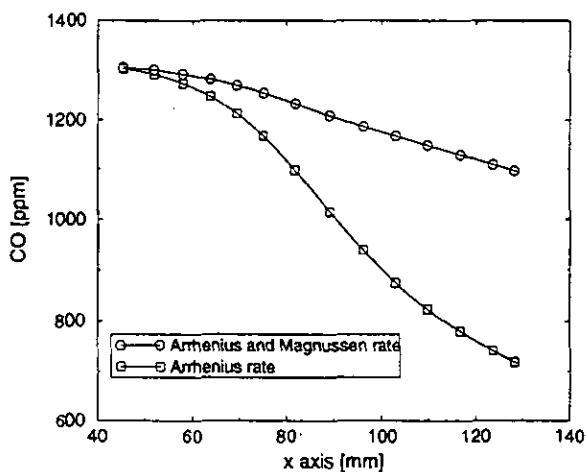


Figure 4: CO mole fraction profile along $j = 18$ plane

The recombination of CO to CO_2 during expansion in the nozzle results in heat release. Thus, the temperature decreases less rapidly than if non reactive flow is assumed. The computed temperature difference at the outlet between the two types of flow is denoted ΔT . Fig. 5 shows the variation of ΔT along the central $j = 18$ plane. As expected, the temperature difference computed using only Arrhenius rates is greater than that obtained assuming Magnussen theory. This temperature difference exceeds 4 K at the nozzle exit in all cases and leads to a modification of the gas stream flow characteristics, which in turn modifies the gas turbine

performance, as discussed by the authors in a separate paper [5].

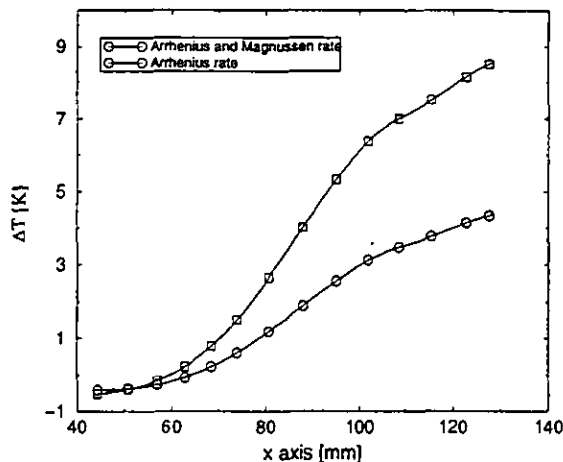


Figure 5: ΔT along $j = 18$ plane

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 ΔT profiles for the following three x 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:

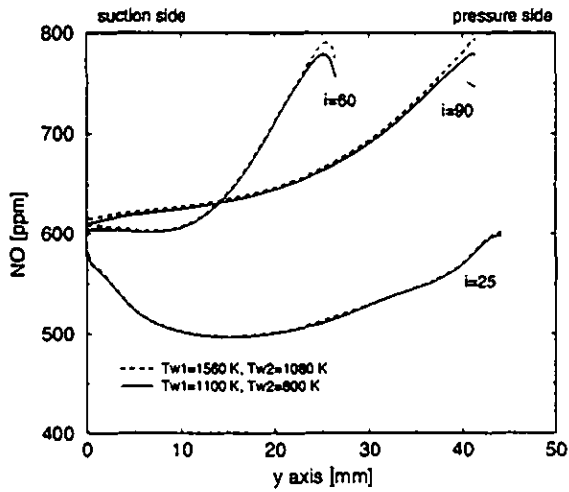


Figure 6: *NO* mole fraction profiles

- 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.

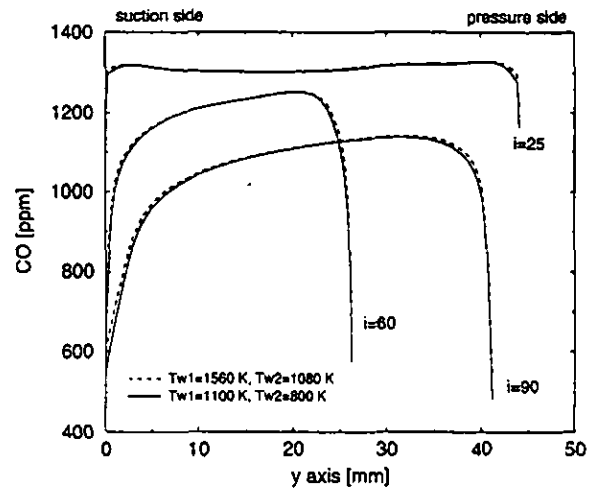


Figure 8: *CO* mole fraction profiles

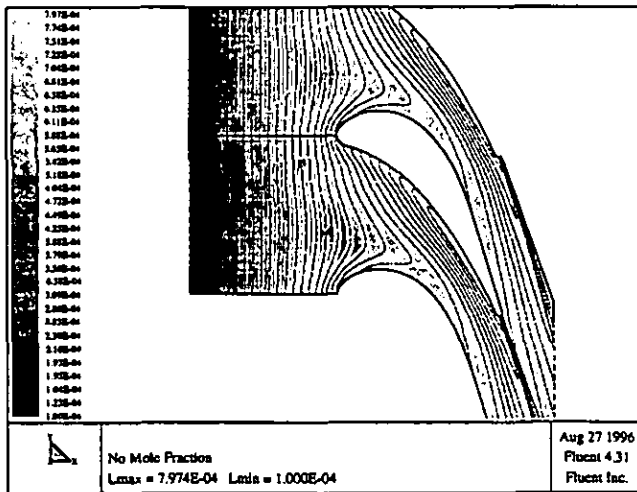


Figure 7: *NO* mole fraction contours

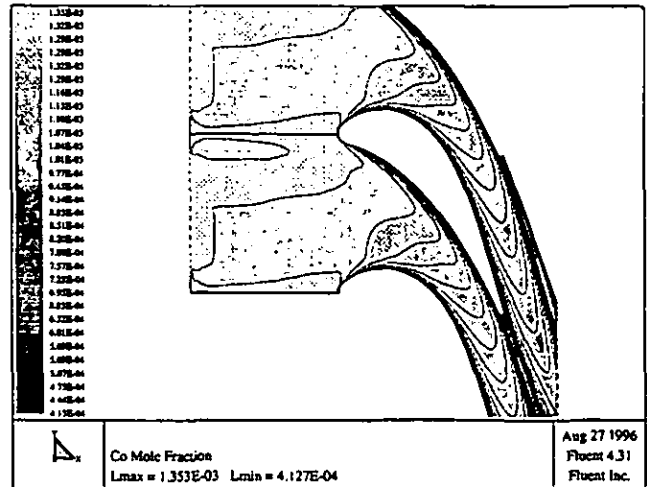


Figure 9: *CO* mole fraction contours

As discussed previously, this recombination of *CO* to *CO*₂ releases a considerable amount of heat. Fig. 10 presents ΔT profiles for three *x* locations and two blade wall temperature distributions. We again note the

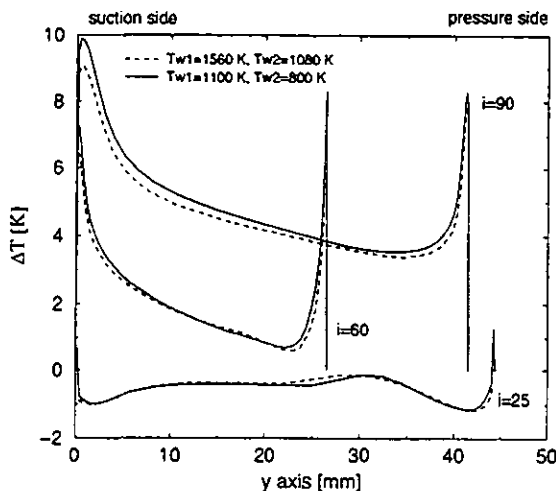


Figure 10: ΔT profiles

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.

Acknowledgments

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