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Emissions from Gas Turbine Combustors

(Part 2, Analytical Model and Numerical Analysis)*

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An axi-symmetrical, two-dimensional model of gas turbine combustors of can-type has been developed in which both turbulent diffusion and chemical reactions of finite rate are taken into account simultaneously. On the basis of this model, the distribution maps of the velocities, temperatures, equivalence ratios and the concentrations of oxygen and nitric oxide, as well as the axial profile of combustion efficiency were predicted numerically, which have several features common with the observed ones. This suggests the availability of the present model for examining the roles of various parameters in the formation process of nitric oxide. Its capacity in predicting the blowout behaviors of combustors was also anticipated.

1. Introduction

In response to an increasing interest in the emissions from gas turbines and jet engines, a number of analytical models of gas turbine combustors have been reported.^{(1)~(9)} Most of them, however, are essentially reactor models in which the marked multidimensionality of the flow field and the considerable nonuniformity in radial profiles of the temperature and species concentrations within a combustor⁽¹⁰⁾⁽¹¹⁾ are taken into account only indirectly in terms of the probability density functions of the equivalence ratio and residence time.

Since the kinetics of nitric oxide formation is highly sensitive to the local temperature and concentration of oxygen, the emission of nitric oxide can not be predicted adequately unless the detailed distribution maps of these quantities and the loci of gas particles are known. In order to meet this requirement economically, a simplified mechanistic model has been developed in which a special parabolizing technique is employed together with moderate use of empirical parameters.

The flow field in a gas turbine combustor is so complicated that no exact mechanistic approach, fully theoretical and tractable by the present numerical technique, seems to be realistic. It appears, therefore, to be a good strategy to examine the fundamental mechanism of pollutant formation and flame stabilization in a gas turbine combustor using an adequately simplified analytical model.

In the present model, the jets of secondary and dilution airs are replaced by the effusions of air through the permeable bands in the liner, and the reverse flow region in the primary zone is treated separately as a well-stirred reactor covered with a hypothetical permeable wall through which burning gas recirculates.

Two-dimensional distribution maps of velocities, temperatures, equivalence ratios and nitric oxide obtained on the basis of this model are in fundamental agreement with the observed ones reported in the previous paper.⁽¹¹⁾ In addition, some insight into the mechanism of flame stabilization is obtained.

2. Nomenclature

A/F	: Air-fuel ratio
E	: Activation energy
EI	: Emission index
F	: Preexponential factor
G	: Mass flow rate
h	: Enthalpy
h_s	: Stagnation enthalpy
i	: Stoichiometric mass ratio of oxygen to fuel
K	: Constant in Eq.(8)
$K_{p,0}$	: Equilibrium constant for the reaction $1/2 O_2 \rightleftharpoons O$
k_1, k_{-1}, k_2, k_{-2}	: Rate constants
k_H	: Constant in Eq.(8)
L	: Length of the combustor
M	: Molecular weight
m	: Mass fraction
p	: Pressure
R	: Rate of generation
$\bar{m}$	: Universal gas constant
r	: Radial distance
r_C	: Radius of the combustor
T	: Temperature
T_i	: Inlet air temperature
u, v	: Axial and radial components of velocity
x	: Axial distance
y	: Radial distance either from the

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boundary of the reverse flow region
 $(x \leq x_R)$ or from the axis $(x > x_R)$
 ε : Constant in Eq.(9)
 η : Combustion efficiency
 θ : Half angle of the spray cone
 μ_{eff} : Effective viscosity
 ρ : Density
 $\sigma_{h,eff}$: Effective Prandtl number
 $\sigma_{m,eff}$: Effective Schmidt number
 ϕ : Equivalence ratio
 $\varphi = m_{ox} - im_{fs}$: Combined mass fraction
 ψ : Stream function

Subscripts

f_u : Fuel
 NO : Nitric oxide
 ox : Oxygen
 pr : Combustion products (or nitrogen)
 o : Overall
 p : Primary zone
 R : Reverse flow region

3. Analytical model

A typical gas turbine combustor of can-type is shown schematically in Fig.1. The primary air is introduced into the combustor through the swirler installed around the fuel injection nozzle, while the secondary and dilution air are introduced through the rows of air holes in the liner. Flame is stabilized by the recirculating flow located at the center of the primary zone.

The analytical model is shown in Fig.2. The mixture of a gaseous fuel and a part of the primary air is introduced into the combustor from its upstream end at mass flow rates of G_{bf} and G_{ba} , respectively, the rest of the primary air being introduced around the mixture stream coaxially at a mass flow rate of G_c . The secondary and dilution airs are effused through the permeable bands in the liner instead of being injected through the air holes.

In order to simulate a conical spray, it is assumed that a fresh mixture is not ignited in the region upstream of the conical surface corresponding to the spray contour.

The reverse flow region located at the center of the primary zone is covered with a hypothetical cylinder, transparent to heat and species, and two permeable cones attached to it at both ends. A recirculating flow is formed around this region by

Fig.1 Gas turbine combustor of can-type

effusing out and taking in the burning gas through upstream and downstream cones, respectively. Flame is stabilized by this recirculating flow. Small fraction of the fuel and the air effused through the first permeable band are taken directly into the reverse flow region at mass flow rate of G_{Af} and G_{AH} , respectively. This region is treated independently as a well-stirred reactor. Combustion efficiency of the reverse flow region is estimated from experiments on well-stirred reactors.^(1,2)

The following assumptions are introduced;

(1) No reverse flow appears and the boundary layer approximation is applicable except in the reverse flow region.

(2) The combustion reaction is of one-step, to which Arrhenius rate law in terms of the time-mean values of the temperature and species concentrations is applicable.

(3) The combustion reaction does not proceed exceeding the equilibrium state.

(4) Turbulent diffusion predominates over molecular one.

(5) The effects of radiative heat transfer and buoyancy are small.

(6) No pressure gradient exists in radial direction.

(7) The reactions related to the formation of nitric oxide do not much violate the mass balance between the fuel, oxygen and combustion products.

(8) The effective Lewis number is unity.

Under these assumptions, the conservation laws for mass, momentum, species and energy are written as follows except for the reverse flow region.

$$\frac{\partial \psi}{\partial x} = -\rho v r, \quad \frac{\partial \psi}{\partial y} = \rho u r \quad \dots\dots\dots (1)$$

$$\frac{\partial u}{\partial x} = \frac{\partial}{\partial \psi} \left(r^2 \rho u \mu_{eff} \frac{\partial u}{\partial \psi} \right) - \frac{1}{\rho u} \frac{dp}{dx} \quad \dots\dots\dots (2)$$

$$\frac{\partial m_j}{\partial x} = \frac{\partial}{\partial \psi} \left(\frac{r^2 \rho u \mu_{eff}}{\sigma_{m,eff}} \frac{\partial m_j}{\partial \psi} \right) + \frac{R_j}{\rho u} \quad (j=1, 2, 3) \quad \dots\dots\dots (3)$$

$$\frac{\partial h_s}{\partial x} = \frac{\partial}{\partial \psi} \left(\frac{r^2 \rho u \mu_{eff}}{\sigma_{h,eff}} \frac{\partial h_s}{\partial \psi} \right) + \frac{\partial}{\partial \psi} \left\{ r^2 \rho u \mu_{eff} \left(1 - \frac{1}{\sigma_{h,eff}} \right) \frac{\partial (u^2/2)}{\partial \psi} \right\} \dots\dots (4)$$

Fig.2 Analytical model

In Eq.(3), the suffix j denotes fuel, φ and nitric oxide as $j=1,2$ and 3, respectively. The mass fraction of the other species, oxygen and combustion products (or nitrogen), are calculated from the mass fraction of fuel and φ thus determined using the following relations.[See assumptions (2) and (7).]

$$m_{os} = \varphi + i m_{fs} \dots\dots\dots (5)$$

$$m_{pr} = 1 - m_{fs} - m_{os} \dots\dots\dots (6)$$

The local equivalence ratio can be estimated from φ using the following relation.

$$\Phi = (1 - \varphi/m_{os}^0)/(1 + \varphi/i) \dots\dots\dots (7)$$

where m_{os}^0 is the mass fraction of oxygen in fresh air.

The effective viscosity μ_{eff} is assumed to be uniform in a cross section. Although the oblique jets of the secondary and dilution air are replaced by the effusions through permeable bands, the effective viscosity is estimated from the following empirical relation which is originally developed by Gosman et al.⁽¹³⁾ and modified by the authors considering the stirring effects of the oblique jets in order to examine the effect of intense turbulent diffusion on the processes of combustion and pollutant formation.

$$\mu_{eff} = K r_c^{2/3} L^{-1/3} \rho^{2/3} \{ (G_{Bc} + G_{Bf}) u_B^2 + G_c u_c^2 + k_H \sum_i (G_{Hi} u_{Hi}^2) \}^{1/3} \dots\dots\dots (8)$$

where K and k_H are empirical constants. For u_B , u_c and u_{Hi} 's in the above equation, the actual velocities with which air passes through the swirler and the liner slit or holes, respectively, of the model combustor reported in the previous paper⁽¹¹⁾ are substituted for the values of the analytical model. Sigma which appears on the right hand side of Eq.(8) denotes a summation pertaining to the air holes located upstream of the cross section in question, while k_H denotes a coefficient taking into consideration the difference between oblique and axial jets in contribution to the effective viscosity.

The generation rate of φ which appears in Eq.(3) is always zero from the definition of φ . The generation rate (negative reaction rate) of fuel is represented by the relation

$$R_{fs} = -\epsilon F p^2 m_{fs} m_{os} \exp(-E/RT) \dots\dots\dots (9)$$

on the basis of assumption (2), where ϵ is the unmixedness factor to take the reaction retard due to large scale mixing into consideration.

For the process of nitric oxide formation, the basic Zeldovich mechanism

was adopted because of its compatibility with the present analytical model.

Assuming the quasi-steady state of nitrogen atoms as well as the partial equilibrium between oxygen molecules and atoms, the generation rate of nitric oxide in Eq. (3) is written as

$$R_{NO} = \frac{2K_{p,O}}{M_{os}^{1/2} M_{pr}} \frac{\rho^{3/2}}{(RT)^{1/2}} m_{os}^{1/2} \times \frac{k_1 k_2 M_{NO}^2 m_{os} m_{pr} - k_{-1} k_{-2} M_{os} M_{pr} m_{NO}^2}{k_2 M_{NO} m_{os} + k_{-1} M_{os} m_{NO}} \dots\dots\dots (12)$$

where k_1 , k_{-1} , k_2 and k_{-2} are the rate constants for the reactions represented by Eq.(10) and (11), whose values are estimated following Baulch et al.⁽¹⁴⁾ The error due to the substitution of nitrogen by the combustion products is less than 34 percent.

4. Numerical analysis

Numerical analysis was carried out following Patankar and Spalding.⁽¹⁵⁾ The combustor cross section was divided into 45 grids except the reverse flow region and the integration step was taken equal to 1/25 of the liner radius except near the points of discontinuous boundary conditions.

The static temperature and species concentrations in the reverse flow region are first assumed, then the numerical procedure is started. When calculation has proceeded down to the end of the reverse flow region, the state in the region is reestimated from the balances of enthalpy and species taking their production and exchange through the hypothetical wall into consideration. The combustion efficiency of the reverse flow region is taken equal to that of a well-stirred reactor.⁽¹²⁾ If the reestimated values coincide with those assumed first, the numerical procedure is proceeded downstream. If not, the procedure returns to the first step.

One of the drawbacks of the present analytical model is that it contains empirical parameters, especially pertaining to the reverse flow region (x_R , r_R , G_A , G_{Af} and G_{AH}). However, viewed from a different stand point, this may be a merit, since it is almost impossible at the present stage to predict the above parameters fully theoretically because of the extremely complicated behaviors of the swirling flow and oblique jets. Only the use of empirical parameters may therefore make realistic prediction possible. In this context, the present model is thought to be a hybrid of a mechanistic and a modular model. The empirical parameters are estimated from cold flow experiments as well as from the

semi-empirical relation of Roberts et al.⁽⁴⁾ and Aiba and Suzuki's experiment.⁽¹⁶⁾

In the numerical analysis, propane vapor is employed as the fuel. The thermodynamic properties and reaction parameters used are shown in Table 1.

5. Results and discussion

Numerical analysis has been executed for a model combustor almost the same in size and shape as the one used for the experiment in the previous paper.⁽¹¹⁾ The operating parameters and estimated quantities employed are tabulated in Table 2.

Typical examples of the predicted distribution maps of the temperatures, equivalence ratios and concentrations of nitric oxide are shown in Fig.3. The fuel flow rate, G_f ($G_{Af} + G_{Bf}$) is taken equal to 1.2 g/s. A high temperature region appears around the axis from downstream half of the primary zone to the upstream half of the secondary zone, where the equivalence ratio is close to unity. Nitric oxide has a peak in concentration on the axis in the secondary zone. This peak is located just downstream of the high temperature region, where the equivalence ratio is approximately 0.9. Nitric oxide, however, shows a relatively a low concentration in the near-wall region even for almost the same temperature and equivalence ratio. This implies that the process of nitric oxide formation is governed by

the history experienced by a gas particle as well as its local state. Therefore, both the flow pattern and the distribution maps of temperatures and species concentrations are important for the discussion on nitric oxide emission.

For convenience of the examination of the validity of the present analytical model, the counterparts of Fig.3 obtained experimentally in the previous paper⁽¹¹⁾ are again shown in Fig.4, although the direct comparison between both figures is impossible since the type of fuel and the ways of introduction of fuel and air are different in each case.

The distribution patterns of the temperature, equivalence ratio and nitric oxide show excellent similarities between Figs.3 and 4 especially in the downstream half of the combustor. This fact suggests that both the model combustor for experimental use and the present analytical model have common characteristics in their flow patterns and mixing and reaction processes, and that, therefore, basic examination of the processes of nitric oxide formation and flame stabilization are possible using the present analytical model.

Table 2 Specifications and operating conditions

Length of the combustor	L mm	350
Radius of the combustor	r_c mm	30
Overall air-fuel ratio	$(A/F)_o$	65
Primary air-fuel ratio	$(A/F)_p$	11
Inlet air temperature	T_i K	300
Operating pressure	p atm	1
Half angle of the spray cone	θ °	40
Effective Prandtl number	$\sigma_{h,eff}$	0.86
Effective Schmidt number	$\sigma_{m,eff}$	0.86
Length of the recirculation zone	x_R mm	55
Radius of the recirculation zone	r_R mm	10
Combustion efficiency in the recirculation zone	η_R	85
Constant in Eq.(8)	K	0.3
Constant in Eq.(8)	k_H	10
Constant in Eq.(9)	ϵ	1

Fig.3 Predicted distribution maps
 $(A/F)_o = 65$, $(A/F)_p = 11$, $T_i = 300$ K,
 $G_f = 1.2$ g/s.

Table 1 Properties of species

		Oxygen	Nitrogen	Propane
Specific heat	J/kg K	862.8+0.2292T	934.7+0.2359T	1874+2.817T
Lower heat value	J/kg	—	—	4.637×10^7
Stoichiometric mass ratio of oxygen to fuel		—	—	3.629
Preexponential factor	kg m/N ² s	—	—	0.5
E/R	K	—	—	19000
Enthalpy	J/kg	862.8T+0.1146T ² -2.673×10 ⁵	934.7T+0.11795T ² -2.890×10 ⁵	1874T+1.4085T ² +4.570×10 ⁷

The predicted temperature (Fig.3) is in excellent agreement with the observed one (Fig.4) in the downstream half of the combustor. The major cause of the discrepancy in the upstream portion is the differences between both combustors in shape, fuel type and introduction of fuel and air. However, droplet collision to the thermocouple, radiative and conductive heat losses from the thermocouple, assumption of one-step reaction and ignored fluctua-

tions in temperature and species concentrations are also the causes of the discrepancy.

Meanwhile, the predicted equivalence ratio (Fig.3) is considerably lower than the observed one (Fig.4) in the upstream portion of the combustor. This may be ascribed to the unvaporized droplets penetrating a considerable distance as well as to the difference in axial profile of air introduction between both combustors.

As for nitric oxide, an excellent agreement is obtained between the predicted distribution map (Fig.3) and the observed one (Fig.4) except in the primary zone. This fact seems to imply the effectiveness of the mechanistic approach as well as the usefulness of the basic Zeldovich mechanism for rough prediction of the emission of nitric oxide.

Figure 5 shows the predicted radial profiles of the velocity, temperature, equivalence ratio and species concentrations. Flame has already spread over the cross section at $x=40$ mm, and almost all oxygen has been consumed. This rapid consumption of oxygen is unrealistic and probably comes from an incomplete eddy mixing (so called "unmixedness") ignored in the

Fig.4 Experimental distribution maps
(A/F)_o = 66, (A/F)_p = 10.6, T_i = 320 K,
 G_f = 1.2 g/s.

(a) $x = 40$ mm

(b) $x = 120$ mm

Fig.5 Predicted radial profiles
The operating condition is the same
as in Fig.3.

Fig.6 Effect of the inlet air temperature

Fig.7 Effect of the operating pressure

Fig.8 Effect of the overall air-fuel ratio

present model. At $x=120$ mm, diffusion burning is taking place between the mixture with oxygen exhausted and the effused fresh air. Although the same situation may be observed around the oblique air jets in practical combustors, the premixedness should be more extensive there.

Figure 6 shows the effects of the inlet air temperature on the profiles of the concentration and emission index of nitric oxide along the axis. The fuel flow rate is kept constant as the inlet air temperature is raised. The peak in nitric oxide concentration is located around $x=150$ mm, while its emission index increases down to this peak, thereafter being kept almost constant. This implies that the formation and decomposition reactions of nitric oxide are frozen around $x=150$ mm, and that its decrease in concentration is caused only by dilution. The peak concentration of nitric oxide increases as the inlet air temperature is raised, consequently its emission index being increased in similar proportion. This suggests an important role played by the primary zone in nitric oxide formation.

The effects of the operating pressure on the profiles of the concentration and emission index of nitric oxide along the axis are illustrated in Fig. 7. The peak in concentration of nitric oxide becomes considerably higher and moves upstream as the operating pressure is raised. Accordingly, the emission index increases markedly. This is principally the result of the stream velocity being decreased by the raised operating pressure, since the fuel flow rate and overall air flow rate are

kept constant. The effect of the raised pressure itself, however, is not small.

Figure 8 represents the variation in axial profile of the concentration and emission index of nitric oxide as the overall air-fuel ratio is raised with the fuel flow rate kept constant. Although the peak in concentration and the ceiling value of emission index are lowered and the peak position advances upstream as the overall air-fuel ratio is increased, their variations are not remarkable.

As shown in Fig. 9, the influences of the primary air-fuel ratio are somewhat different from the above. The peak in concentration of nitric oxide moves downstream as the primary air-fuel ratio is lowered, being located in the secondary zone when the primary air-fuel ratio is richer than the stoichiometric. The height of the peak and the emission index of nitric oxide, on the other hand, show their maximum at the stoichiometric primary air-fuel ratio. This behavior of nitric oxide corresponds well to that of the temperature.

In the course of numerical analysis, an extinction of flame is frequently experienced especially when an excessively large effective viscosity is employed. This fact seems to imply the capability of the present analytical model to predict the blowout behaviors of gas turbine combustors.

6. Conclusions

An axi-symmetrical, two-dimensional mechanistic model of gas turbine combustors of can-type has been developed introducing a special parabolizing technique. The distribution maps of the temperatures, equivalence ratios and species concentrations as well as the axial profiles of the combustion efficiency have been obtained numerically. The conclusions obtained are as follows.

(1) The combination of the basic Zeldovich mechanism and the assumptions of one-step combustion reaction, the quasi-steady state of nitrogen atoms and the partial equilibrium between oxygen atoms and molecules presents distribution maps of nitric oxide in qualitative agreement with the observed ones especially in the downstream half of the combustor. This fact suggests the capability of the present analytical model to examine the influences of various factors on the emission of nitric oxide.

(2) A major fraction of nitric oxide is produced in the primary zone and the upstream half of the secondary zone. The primary air-fuel ratio, therefore, has an effect far greater than the overall air-fuel ratio on the emission of nitric oxide. The emission of nitric oxide also increases as either the inlet air temperature or operating pressure is raised.

(3) The capability of the present analytical model to predict the blowout

Fig. 9 Effect of the primary air-fuel ratio

behaviors of gas turbine combustors is anticipated.

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