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ABSTRACT

NOx emission control by water injection on a staged turbine combustor (STC) was modeled using the KIVA-II code with modification. Water is injected into the rich-burn combustion zone of the combustor by a single nozzle. Parametric study for different water injection patterns was performed. Results show NOx emission will decrease after water being injected. Water nozzle location also has significant effect for NO formation and fuel ignition. The chemical kinetic model is also sensitive to the excess water. Through this study, a better understanding of the physics and chemical kinetics is obtained, this will enhance the STC design process.

INTRODUCTION

To develope an ultra-low NOx emission combustor for next generation gas turbine, lots of concepts are under study. Water injection, which was regarded as an impractical way, is being proposed again. It is clear that NOx formation rate is highly dependent on the flame temperature. A decrease in flame temperature will reduce the formation of NO. In this study, water injection is modeled using the KIVA-II[1] CFD code for a staged turbine combustor (STC). This approach offers more insight into the physics of the flow and the chemical kinetics involved.

The STC under study consists of a rich-burn (RB) zone and a lean-burn (LB) zone. These two zones are connected by a quick-quench (QQ) section, see Fig.1. An air assist fuel nozzle is located at the inlet of the RB zone. This nozzle has two fuel injection passages and four air flow passages. The van angle of the middle, outer, and dome air flow passages are 61.3°, 60.2°, and 60.2°, respectively (Fig.2). Detail of the operating condition will be given later. This study is concentrated on the RB section, which is critical to the performance of combustor.

Literature review showed that the water injection method is still in use widely in industrial stationary gas turbine[2]. For the aircraft engine, some experimental studies were done in the early 70s[3,4]. The results are very impressive. Visser and Bahlmann proposed an empirical model for the water injection of NOx abatement emission control[2], which is based on the operating data collections. A detail of the experimental configuration and study was recorded by Klapatch and Koblish[3]. KIVA-II[1] has been using in gas turbine combustor simulation for some years[5-7]. The code was modified to fit the special geometry and inlet boundary conditions for gas turbine combustor. Because the original KIVA-II code can only handle one liquid spray besides inflow air, modifications are needed for modeling fuel and water sprays simultaneously. In this study, a simplified propane chemical kinetics model[8] is used for modeling Jet-A fuel chemical reaction in gas phase. The water injection effect on this model will be discussed. Qualitative comparison of the effects of different water injection and the associated emission issues will be presented.

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DESCRIPTION OF PROBLEM

The nozzle and primary zone of the RB section is shown schematically in Fig. 2. The two fuel injectors are located at the center of the RB inlet. Water is injected into this section only. At inlet, the following conditions were used:

- Air temperature = 1000F (811k);
- Ambient pressure = 90psia (6.2×10^6 dyn/cm^2);
- Air mass flow rate = 1.09lbm/sec(494.4 g/s);
- Air flow split = 7.8/19.1/25.5/47.6% (from inner to dome);
- Air flow passage area = 0.007/0.0117/0.0156/ 0.027 ft.^{2} (6.50/10.87/14.49/25.08cm^2);
- Equivalence ratio =2.0;
- Fuel split 50%/50%;
- Turbulent length scale = 0.25 of the respective flow passage width;
- Turbulent kinetic energy = 1% of the respective 0.5 W^2.

where W is the mean axial velocity at the inlet. These conditions are similar to the operating conditions encountered in the advanced combustion systems.

The inlet boundary conditions are the specification of the density (calculated from the temperature and pressure given above) and W (from the mass flow rates and flow areas given above). The radial velocity was set so that the inlet flow is tangential to the flow passages. The exit boundary condition is to specify the pressure. The combustor walls are assumed to be adiabatic.

Water is injected at locations (N1, N2, N3 and N4 in Fig.2) around the flame front in the primary zone. Only mono-injector was used. Water/Fuel mass flow rate ratio (hereafter, W/F will be used) is taken as 1/8, 1/4, and 1/2. During the numerical simulation, water injection is not started right from the beginning but after the steady state condition is reached. After turning on the water injector, a solution is considered to be convergent when the code is continuously run until another steady solution is achieved.

SOLUTION OF PROBLEM

The problem is modeled as a turbulent reactive flow and is closed by the κ–ε model with wall functions. Due to the geometrical and physical symmetry, the problem is treated as axisymmetic with swirl.

Numerical Details

This study is performed using a modified version of KIVA-II. This code is capable of solving 2D/3D transient turbulent chemical reactive flow with a single component vaporizing fuel spray. The numerical scheme is base on the Arbitrary-Lagrangian-Eulerian (ALE) method[9]. A stochastic particle method is used to calculate the liquid sprays. Submodels for droplet distortion, breakup, collision, coalescence and oscillation are supplied. Several upwind convection schemes are included. Standard κ–ε model and subgrid model are also available.

The computational grid for RB zone was generated by an elliptical method and is shown in Fig.3. It has 67x50 computational cells.

Code Modifications

KIVA-II is written specially for IC engine research, and the ability of handling complex geometry is limited (this is not the case for the newly released KIVA-3 code). To model STC problem, modifications are needed. The major modifications include:

1. Changing the inlet boundary condition to enable the code for handling the four inflow air passages;
2. Updating wall boundary conditions to allow arbitrary shaped combustor wall;
3. Adding water injector to the code so that it can inject fuel and water at the same time, since the original code can not inject two different liquids simultaneously;
4. Modifying the code to output the species and flow pattern information;
5. Calculating the emission index, which is defined as the ratio of the grams of pollutant formed divided by the kilograms of fuel consumed.

As mentioned, KIVA-II has very comprehensive submodels for the fuel injection. The added water injector and the corresponding supporting subroutines are directly borrowed from the KIVA-II fuel spray model with some minor changes and simplifications. Assumptions used in this modification are:

1. There is no interaction between water droplets and fuel droplets;
2. Turbulent influence on water droplets is ignored;
3. Water droplet distortion, breakup, collision, coalescence and oscillation submodels are

turned off.

In the current work, water is injected directly to the RB primary zone. Numerical experiments show that, first, no fuel droplets are found in the primary zone after the steady operation state has been achieved. All droplets have vaporized before coming to the primary zone. Second, the water droplets are vaporizing so fast that most of them can only stay in the liquid phase for about 1~3 timesteps (about 10^{-6} second). Accordingly, the droplet transportation behavior can be ignored. Due to two different liquid (water and fuel) source terms in the governing partial differential equations, the code needs a much smaller time step size for stability. A two-order-of-magnitude timestep size reduction is usually needed for simulation with water injection included. The timestep size for single fuel injection is about 10^{-4} second. The physical/chemical properties of water are taken from KIVA-3[10].

Chemical Kinetics

A simplified Jet-A fuel chemical kinetic model[8] is used. It includes six equilibrium reactions:

(1) $H_2 \leftrightarrow 2H$

(2) $O_2 \leftrightarrow 2O$

(3) $N_2 \leftrightarrow 2N$

(4) $O_2+H_2 \leftrightarrow 2OH$

(5) $O_2+2H_2O \leftrightarrow 4OH$

(6) $O_2+2CO \leftrightarrow 2CO_2$

and five kinetic reactions:

(7) $C_3H_8+(3/2+8/4)O_2 \leftrightarrow 3CO+4H_2O$

$$K_f=10^{12}Exp(-15106/T)[C_3H_8]^{0.1}[O_2]^{1.65}$$

$$K_b=0$$

(8) $CO+(1/2)O_2 \leftrightarrow CO_2$

$$K_f=3.981\times10^{14}Exp(-20141/T)[CO][H_2O]^{0.5}[O_2]^{0.25}$$

$$K_b=5\times10^{8}Exp(-20141/T)[CO_2]$$

(9) $O+N_2 \leftrightarrow N+NO$

$$K_f=6.008\times10^{13}Exp(-38000/T)[N_2][O]$$

$$K_b=3.27\times10^{12}T^{0.3}[N][NO]$$

(10) $O+NO \leftrightarrow O_2+N$

$$K_f=1.50\times10^{9}TExp(-19450/T)[NO][O]$$

$$K_b=6.3\times10^{9}TExp(-3172.3/T)[N][O_2]$$

(11) $N+OH \leftrightarrow H+NO$

$$K_f=6.30\times10^{11}T^{0.5}[N][OH]$$

$$K_b=1.6982\times10^{14}Exp(-24560/T)[H][NO]$$

This model uses propane in the gas phase and Jet-A properties in liquid phase. Two step mechanism (reactions 7 and 8) is applied to the reaction of propane, and extended Zel'dovich NOx formation mechanism (reactions 9-11) is included. If we ignore the chemical mechanism effected by water injection, and only consider the temperature drop due to heat absorbing, one can see that reaction 9 will have the greatest effect due to its largest activation energy. The model does not include reactions directly between water and CO or NO. But, (1) higher concentration of water will increase CO_2 formation speed at reaction 8, since H_2O has included in K_f; (2) through reaction 5, higher concentration of water will effect O_2 and OH concentration, and thus effect CO and NO formation.

This model is simplified from a benchmark model which has 131 reactions with 45 species[11] with emphasis on NO and CO formations. Excess water was not accounted. In high temperature, how much does excess water involved in combustion kinetics is still uncertain. Further investigations regarding these issues are needed. C.F. Melius et al[12] found that the effect of water at high density and high temperature can be treated as a solvating agent and as a catalyst on the water gas shift (CO oxidation) reaction:

$$CO+(n+1)H_2O \rightarrow HCOOH+nH_2O \rightarrow CO_2+H_2+nH_2O$$

CO oxidation reaction[13] also should be concerned:

$$CO+OH \leftrightarrow CO_2+H$$

This may be a direction for updating current kinetic model. Due to the lack of available experimental data, new model will not be available at this time.

RESULTS AND DISCUSSION

Numerical results were obtained using the quasi-second-order upwind scheme in KIVA-II. Only evaporation model was used for both of the liquid (fuel and water) sprays. The simulation procedure is similar to the gas turbine normal working condition. The code is run 1000 time-steps (about 1.9×10^{-2} second real time simulation) without fuel injection and combustion. Afterward, the fuel injection is turned on along with the ignition. As mentioned, water is not injected until the steady state solution is reached. Results of the case without water injection and W/F=0.5 case for water nozzle located at N3 (see Fig.2) are compared in Fig. 4.

Without Water Injection

The left columns of Fig. 4 show steady-state velocity vectors, temperature field, distribution of the liquid fuel particles and contour plots of the concentration of each species. There are two recirculation zones in the velocity field, one located near the center line and the other at the left upper corner. The size and shape of the center-line recirculation zone has an important influence on the performance of the RB zone[6]. It offers a heat source to evaporate and ignite the incoming fuel droplets. From the isotherm plot, it is seen that there is a high-temperature gradient region right after the isotherm lever 2, and lever A is the highest temperature.

From mass fraction contour of each species, several observations can be made:

1. Due to fuel rich mixing, O_2 has been totally consumed at the very early stage of the chemical reactions. A comparison between O_2 and temperature contour plots shows the similarity of these contours, indicating the location of flame.

2. From the fuel and the N_2 contour plots and the cross reference with the flow field, it is seen that both fuel and air are diffused into the flame and are following the flow field out side the center-line recirculation zone.

3. N_2, NO contour plots and temperature field comparison indicates that (1) the similarity of highest temperature contour lever A with lowest N_2 contour lever 2 shows the influence of high temperature to N_2 dissociation; (2) largest NO concentration is also found at highest temperature zone, but instead of equally distributed in lever A zone, it concentrates at the wall of the converging section.

4. CO formed right after the flame and it also has the highest concentration at highest temperature region.

With Water Injection

Different nozzle locations are shown in Fig. 2 and Table 1. Results of W/F=0.5 case for N3 water nozzle are shown in the right column of Fig. 4. From temperature and H_2O contours, one can find the water nozzle location at temperature contour lever 7 and H_2O contour lever A. Around the nozzle, temperature is much lower and H_2O is the highest. Comparing with no water injection case at left column, we find:

1. Flow fields do not change for these two cases, and areas which have peak temperature contours A and 9 become much smaller for water injection case. Total temperature distribution remains about the same shape except around water nozzle.

2. CO_2 contours do not change much, but concentration of CO drops significantly. From carbon balance and considering the two steps $C_3H_8 \rightarrow CO \rightarrow CO_2$ in reactions (7) and (8), one can see that more fuel are remain unburned in the water injection case. This is due to less heat being carried by recirculation zone after water injected, thus more difficult to vaporize and ignite fuel.

3. Concentrations of N, NO, O, H2, H, N, and OH decrease after water injection, and they are sensitive to the location of water nozzle. This is in good agreement with kinetic theory.

TABLE 1: Water Nozzle Locations

Nozzle*	x	r
N1	0.3 L	0.7 L
N2	0.4 L	0.7 L
N3	0.6 L	0.7 L
N4	0.7 L	0.7 L

* See Fig. 2

Water/Fuel ratio versus NOx emission Water is injected with different W/F ratios from 1/2 to 1/8 using N3 water nozzle. Results show that the water injection does not influence the flow pattern much (almost no change) due to different amount of water injected. The trend of NO lever decreases with increasing W/F is shown in Fig. 5. Before the water injector, emission indexes for different W/F ratios remain the same because water injection only effect downstream flows. At the outlet, W/F = 0.5 could reduce NO emission by about 50%.

Location of nozzle versus NOx emission References 3 and 13 show that water injection may reduce NOx formation by 30~60% when W/F = 2, depending on different injector position. Parametric study for different nozzle locations is given in Table 1 with W/F = 0.5. From Fig. 6, one can see that N2 nozzle gives best NO reduction. Parametric study shows the position of water nozzle will effect the center recirculation zone and the fraction of burning mixture, which is cooled by water. If water nozzle is too close to the recirculation zone, it will have larger influence on fuel evaporation and ignition. It also has less cooling effect to the convergence section, where NO has highest concentration. On the other hand, if water nozzle is too far away from the recirculation zone, less mixture will be influenced by water injection.

CONCLUSIONS

Numerical simulation of the water injection in a staged gas turbine combustor is obtained using a modified KIVA-II code. The code was modified to inject two different liquids simultaneously. It is found that center recirculation zone and chemical kinetics are very sensitive to water injection. However, since more fuel is unburned after water has been injected, a complete study of STC is needed before a firm conclusion can be made. The parametric study of different W/F ratio shows more water will reduce more NO but will leave more fuel unburned, the latter may cause soot and affect the lean burn section. Also, the location of water nozzle is critical to the fuel vaporization, ignition, and combustion kinetics. It has considerable influence on the emission.

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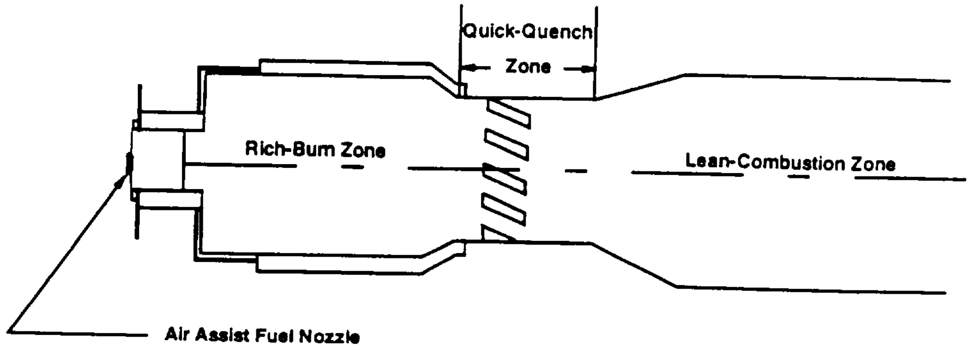


Fig. 1 Schematic Diagram of a Staged Turbine Combustion

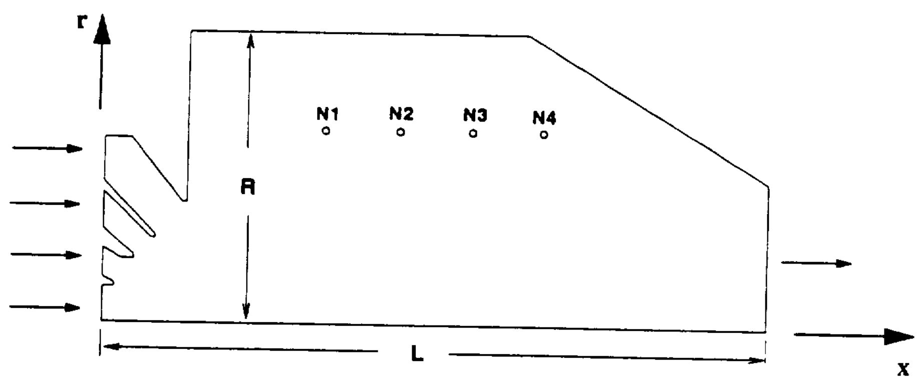


Fig. 2 RB Zone Computational Section (The four air passage nozzle is shown at the left end of the RB zone. The lower and upper passages are the inner and dome air passages, respectively. N1 - N4 are water nozzles)

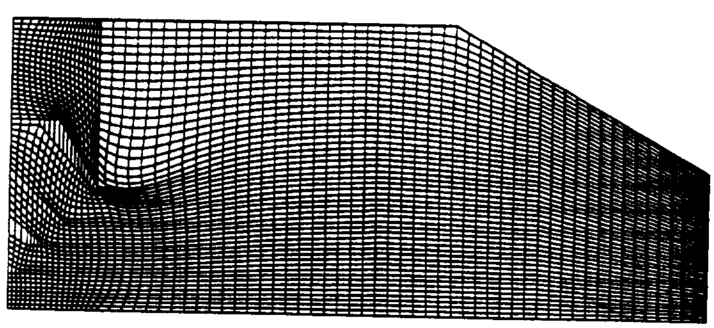
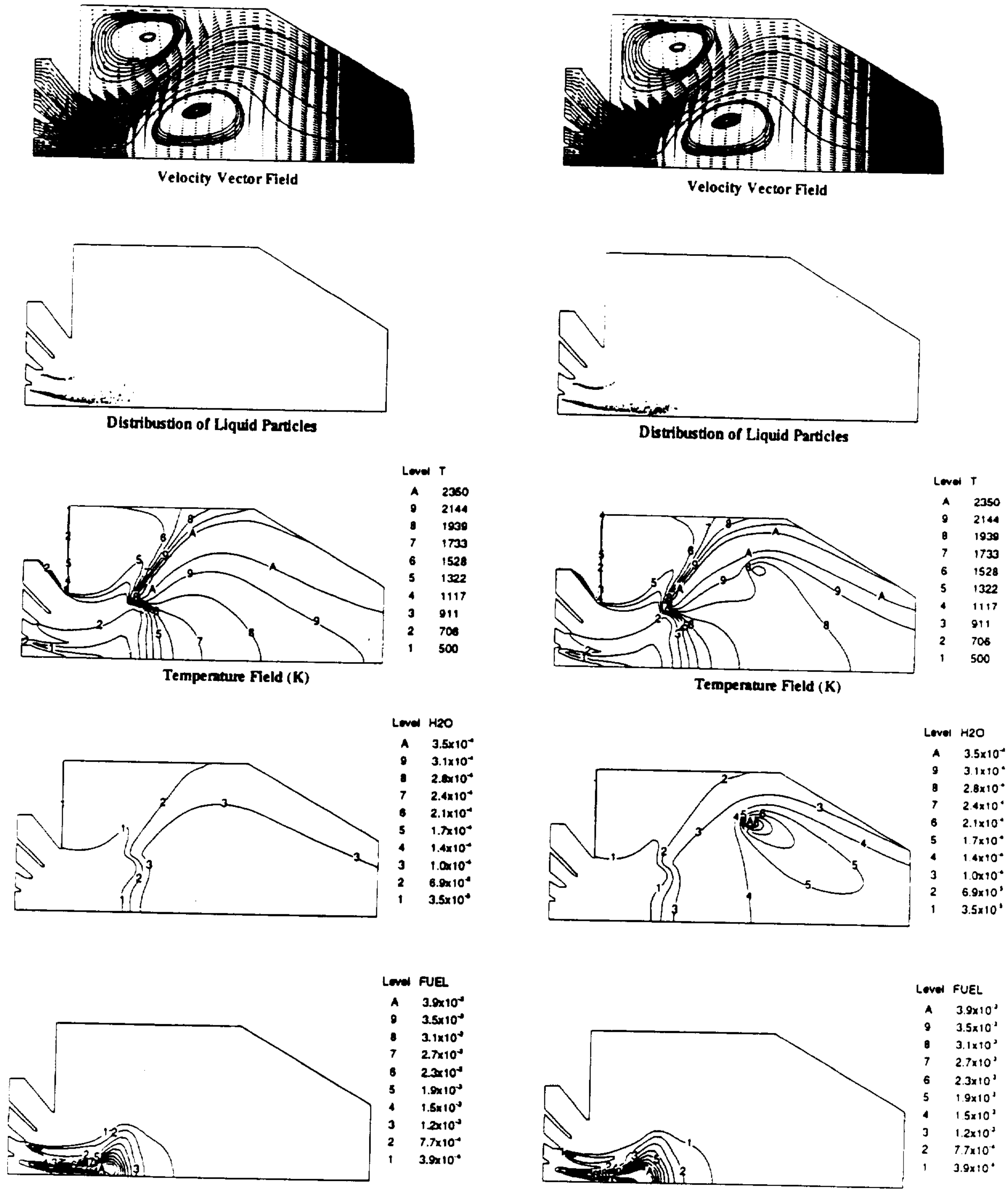


Fig. 3 Computational Mesh of RB Zone



without water injection

with water injection

Fig. 4 Numerical Results of the case without water injection and with water injection

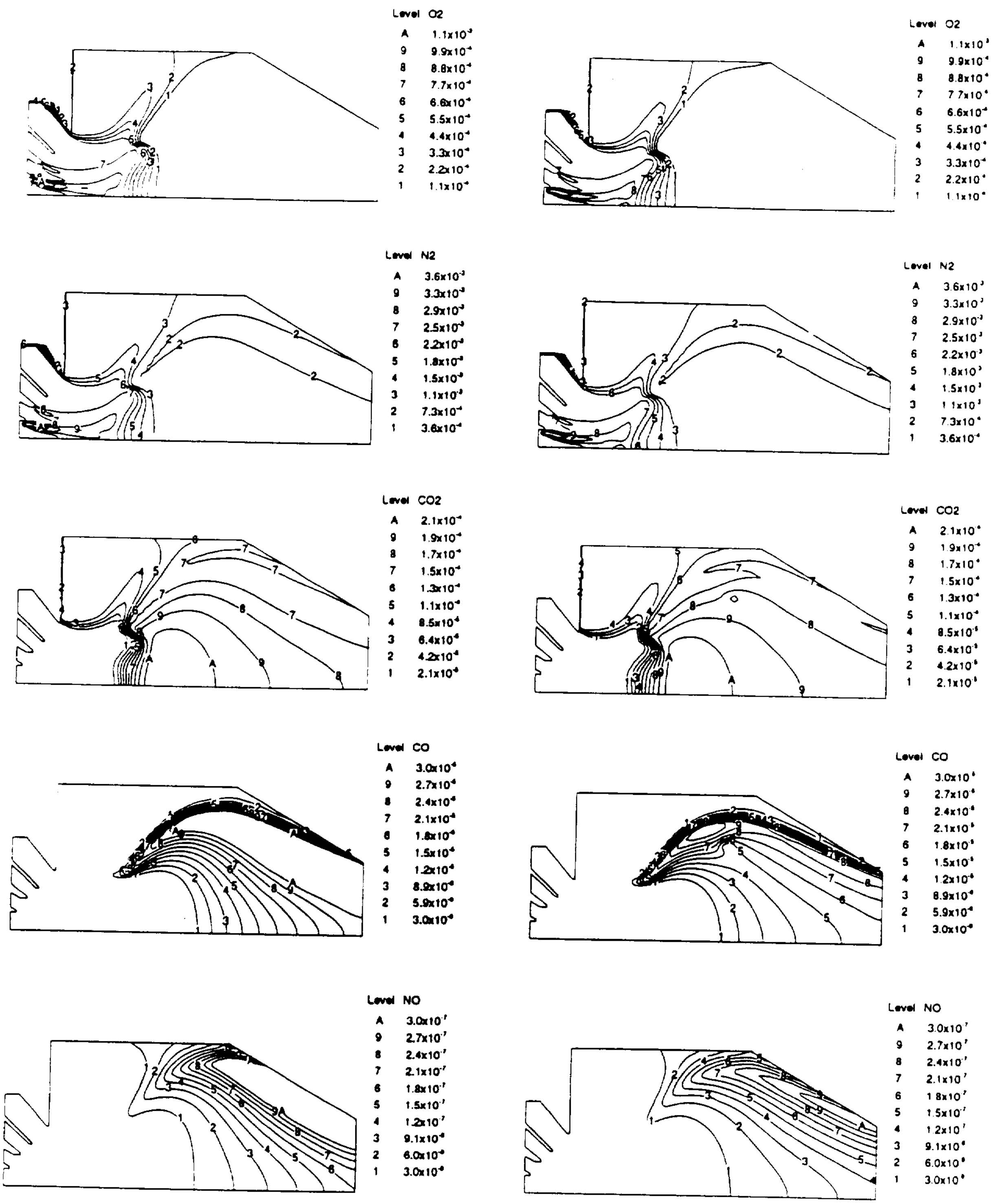
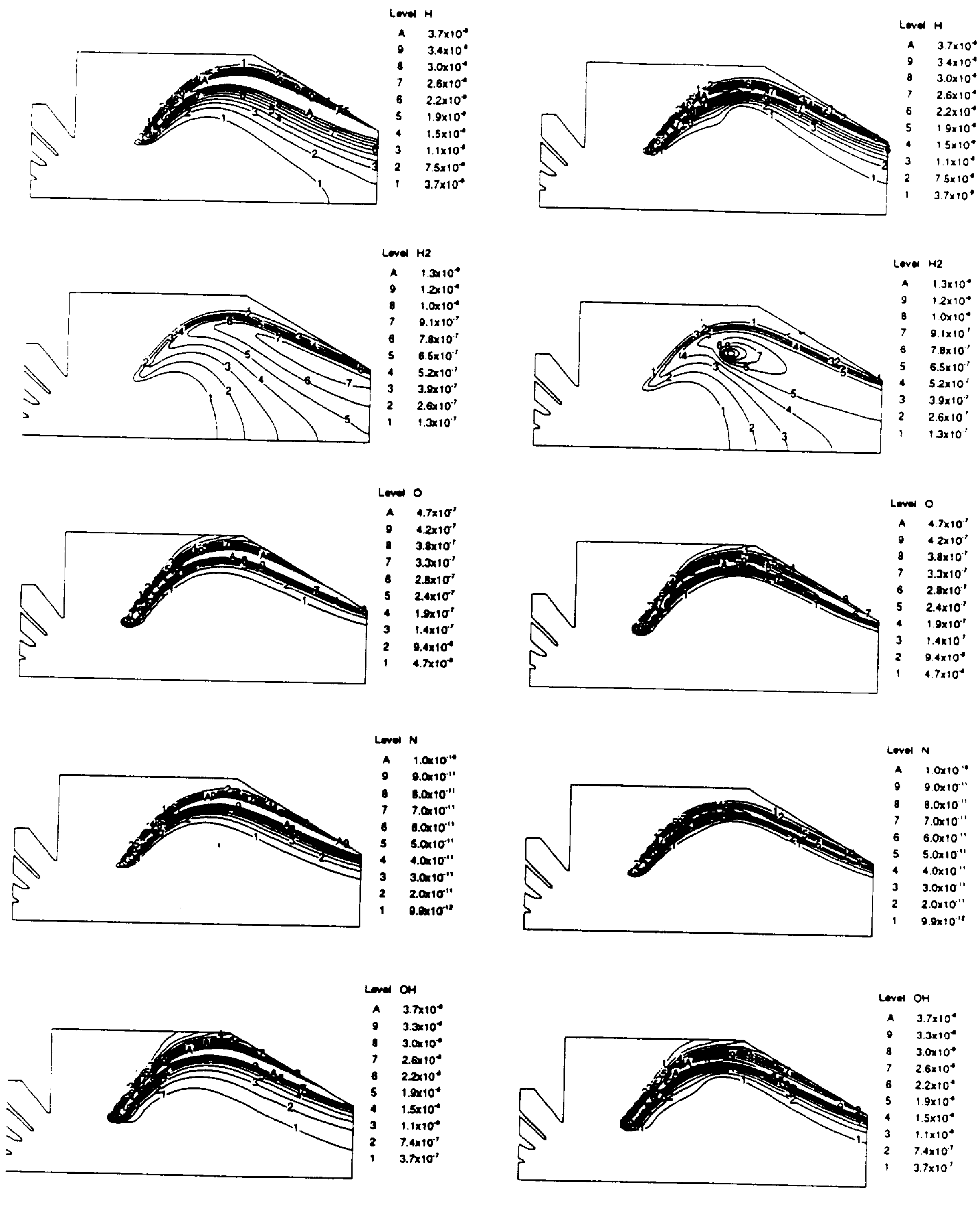


Fig. 4 Numerical Results of the case without water injection and with water injection (continued)



without water injection

with water injection

Fig. 4 Numerical Results of the case without water injection and with water injection (concluded)

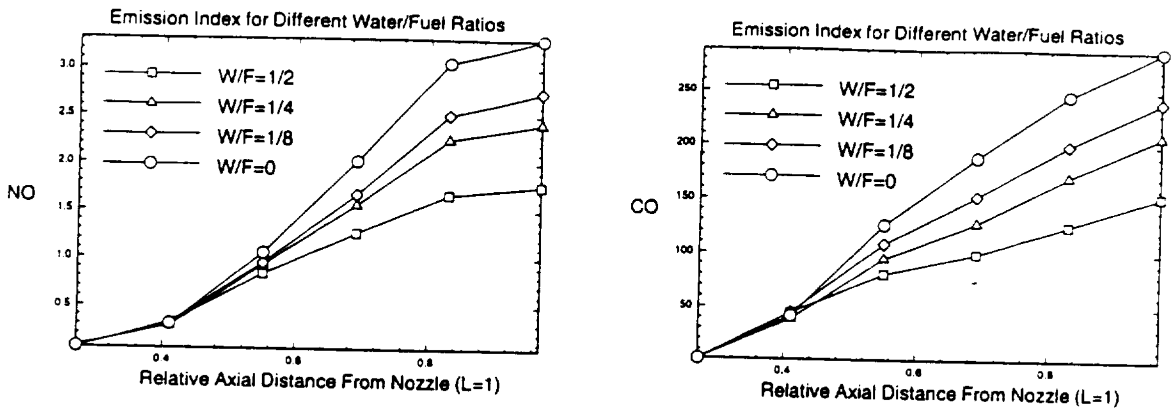


Fig. 5 NO & CO Emissions vs. Water/Fuel Mass Ratio

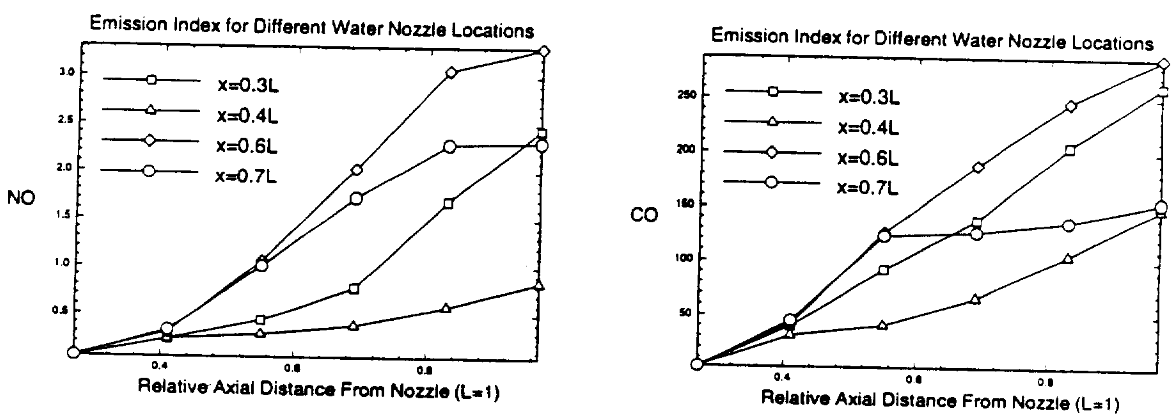


Fig. 6 NO & CO Emissions vs. Water Nozzle Location