NASA-CR-193366

IN-09-CR
176449
p-28

EVALUATION OF CANDIDATE WORKING FLUID FORMULATIONS FOR THE ELECTROTHERMAL - CHEMICAL WIND TUNNEL

Principal Investigator: Dr. Jale F. Akyurtlu

Co-Principal Investigator: Dr. Ates Akyurtlu

FINAL REPORT

for

NAG-1-767

Hampton University
Department of Engineering
Hampton, Virginia

(NASA-CR-193366) EVALUATION OF CANDIDATE WORKING FLUID FORMULATIONS FOR THE ELECTROTHERMAL-CHEMICAL WIND TUNNEL Final Report (Hampton Univ.) 28 p

N93-31848

Unclas

G3/09 0176449

Introduction

A new hypersonic test facility which can simulate conditions typical of atmospheric flight at Mach numbers up to 20 is currently under study at the NASA/LaRC Hypersonic Propulsion Branch. In the proposed research it was suggested that a combustion augmented electrothermal wind tunnel concept may be applied to the planned hypersonic testing facility. The purpose of the current investigation is to evaluate some candidate working fluid formulations which may be used in the chemical-electrothermal wind tunnel.

Work Done

The efforts in the initial phase of this research were concentrated on acquiring the code used by GASL to model the electrothermal wind tunnel and testing it using the conditions of GASL simulation. The early version of the general chemical kinetics code (GCKP84) was obtained from NASA and the latest updated version of the code (LSENS) was obtained from the author Dr. Bittker. Both codes are installed on a personal computer with a 486 25 MHz processor and 16 Mbyte RAM. Since the available memory was not sufficient to debug LSENS, for the current work GCKP84 was used.

The Effect of NO_2 Reactions: As a first step we tried to reproduce the results obtained by GASL for air-argon mixtures. For this purpose the GASL kinetic and thermodynamic data provided in reference (1) are used. Although kinetic constants for reactions involving NO_2 (reactions 6 and 7 in the GASL table) were given in Table 7 of reference (1), it was indicated in the report that these reactions were not considered in the computations. Private communication with O. F. Rizkalla confirmed this and the reason given for the exclusion of these reactions were the unavailability of high temperature thermodynamic data and the expectation that their influence on the test gas composition will be negligible.

We have obtained high temperature thermodynamic data for NO_2

and several other species of importance to our analysis[2]. The data obtained contains two sets of coefficients for the ranges 200 to 1000 K and 1000 to 10,000 K. For some species the upper limit is 20,000 K. Since GASL has used three temperature interval fit for their thermodynamic data, the NO_2 data could not be incorporated to their thermodynamic data, and the McBride data was used in our studies as a complete set.

The initial conditions for the reactive nozzle flow were taken from Table 6 of reference (1). A 5° nozzle with the specified throat area was used. The nozzle area, A in cm^2, is given by

$$A = 0.0240466\, x^2 + 0.198988\, x + 0.41166$$

In our simulations the reactions and accompanying rate data given in Table 7 of the GASL study[1] are used. For some runs the kinetic data for reaction 6 was replaced by the data from a test case supplied by Dr. Bittker with LSENS[3], and the results shown in the second row were obtained using the high temperature kinetic data for reactions 6 and 7 reported by Jachimowski[4]. The result of our simulations are compared with the GASL results[1] in Table 1.

Considering the fact that the GASL results are read from a graph, the NO, O, and O_2 mole fractions have been reproduced by using both the GASL thermodynamic data and the McBride data. In fact, McBride Thermodynamic data appears to produce results closer to those of GASL. The only major discrepancy between our simulations and the GASL results is the nozzle length required to produce an exit Mach number of 16. The nozzle length from Figure 16 of reference 1 is about 8.9 ft while our simulations indicate a nozzle length of about 8.7 m.

The first 6 rows of the table show the effect of NO_2 kinetics on the composition of the gas in the nozzle. The main effect of the NO_2 reactions is on the oxygen atom concentration. When these reactions are excluded from the calculations the oxygen atom mole fraction at the nozzle exit is 1.24E-2 while with the NO_2 reactions the oxygen atom mole fraction falls below 7.25E-5 for all rate data. The effect of NO_2 reactions on the NO mole fraction is not that significant. The NO mole fraction is 4.84E-2 when the reactions are excluded and about 5.6E-2 when they are included.

Table 1. Effect of NO_2 reactions on the test gas composition with air as the working fluid.

Reaction Information	Conditions at 800 cm (y_i in mole frac.)				
	T (K)	y_{NO}	y_O	y_{O2}	M_a
NO_2 Reactions Included GASL Reaction Data	271.66	5.592E-2	5.625E-7	0.1813	15.367
NO_2 Reactions Included Data from Jachimowski	270.90	5.604E-2	7.253E-5	0.1813	15.388
NO_2 Reactions Included Bittker's Data for 6	267.04	5.648E-2	6.883E-14	0.1811	15.477
Reaction 7 Excluded GASL Data for 6	322.81	3.653E-2	2.715E-3	0.1782	14.131
Reaction 7 Excluded Bittker's Data for 6	291.57	3.352E-2	1.387E-3	0.1777	14.910
NO_2 Reactions Excluded McBride Thermo Data	263.20	4.838E-2	1.246E-2	0.1778	15.505
NO_2 Reactions Excluded GASL Thermo Data	260.8	5.106E-2	1.067E-2	0.1776	15.55
GASL Results at Nozzle Exit		4.75 E-2	1.9 E-2	0.173	16.0
NO_2 Reactions excluded McBride Data-Exit Cond.	247.44	4.838E-2	1.244E-2	0.1778	16.00

Simulation Conditions and Procedure: Results have been obtained at Mach 16 free jet conditions for air, air containing 10% ammonia, air containing water equivalent to the hydrogen in 10% ammonia mixture, and a mixture obtained by replacing some nitrogen in air by ammonia to give 10% ammonia. Computations for air and air + 10% NH_3 mixtures were done for 5 and 10 degree nozzles while for the others only a 5 degree nozzle was used. The total enthalpy was

3159.5 cal/g and the mass flow rate was 13302 g/s for all computations. The specified total enthalpy is assumed to be provided by electrical energy input to the feed gas mixture. The mixing chamber pressure was 4690 atm. A lower pressure, 2554 atm, was also tried for air and air + 10% NH_3 mixture. These values were chosen to keep the conditions used in this study similar to the conditions of the GASL study. In all computations reactions involving NO_2 were included and the rate data reported by Jachimowski[4] were used for these reactions. For all the other reactions GASL kinetics[1] were employed.

The computation procedure was as follows:

- Find the initial mixture temperature to give the desired total enthalpy in the mixing chamber. Chemical and thermal equilibrium was assumed to exist in the mixing chamber. The equilibrium conditions and gas composition were found using the equilibrium combustion option of the GCKP.
- Pressure and temperature at the throat are calculated from the reservoir conditions found in the first step using

$$p^* = p_0 \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}} \qquad T^* = T_0 \left(\frac{2}{\gamma+1}\right)$$

  Gas composition at the throat was assumed to be the same as that in the mixing chamber.
- The gas velocity was adjusted to give an initial Mach

number slightly above 1 (usually around 1.025). In some cases, due to the reactions taking place, just after the throat, temperature increases and Mach number decreases and the flow is choked not at the throat but at some distance from it in the expanding section of the nozzle. This necessitates starting Mach numbers even as high as 1.16 at the throat.

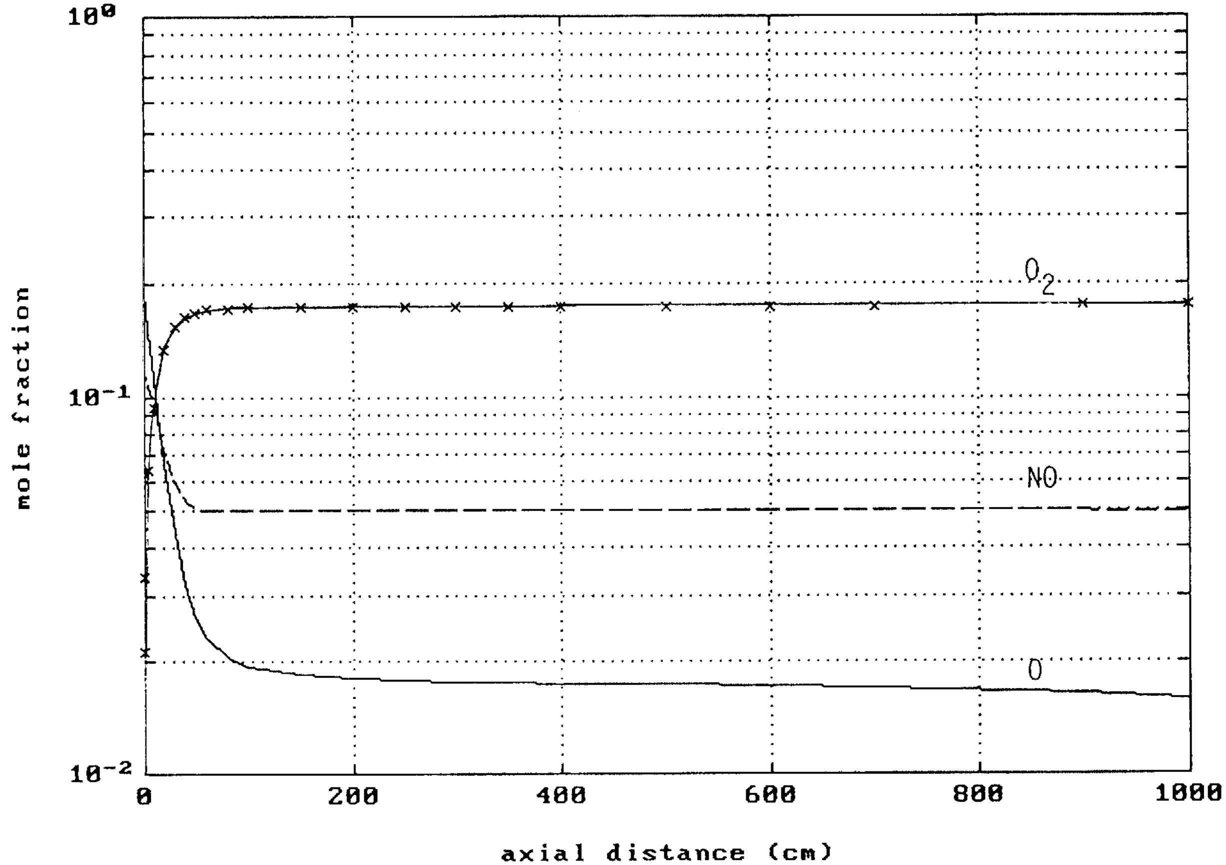
- Adjust the throat area to give the desired mass flow rate.

Results: The results are shown in Figures 1 through 9. In each figure the first chart shows the variation of gas composition up to an axial distance of 1000 cm while the second chart covers the region up to an axial distance of 500 cm and is a blown up version of the first one. The results indicate that for the conditions specified, the flow in the nozzle is essentially frozen beyond 500 cm and for this reason the flow conditions and gas compositions at 500 cm are summarized in Table 2.

The conclusions derived from Table 2 can be summarized as follows:

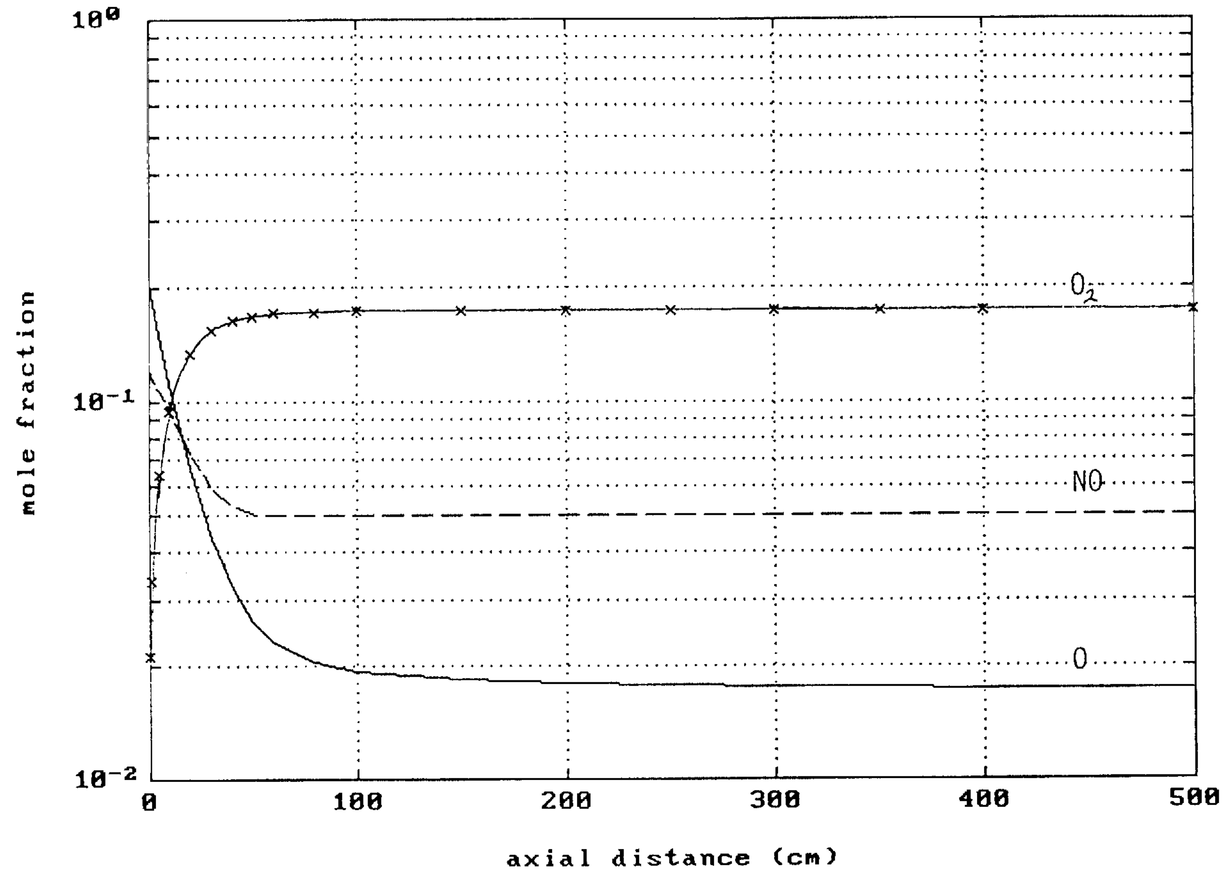
- The addition of NH_3 or H_2O to air decreases the Mach number at the nozzle exit. This is mainly due to smaller γ values of these mixtures. To achieve Mach 16 at the nozzle exit the expansion angle of the nozzle after about 300 cm from the throat should be increased gradually. An initial section with 5 degree expansion is necessary to preserve the high rate of

Figure 1a



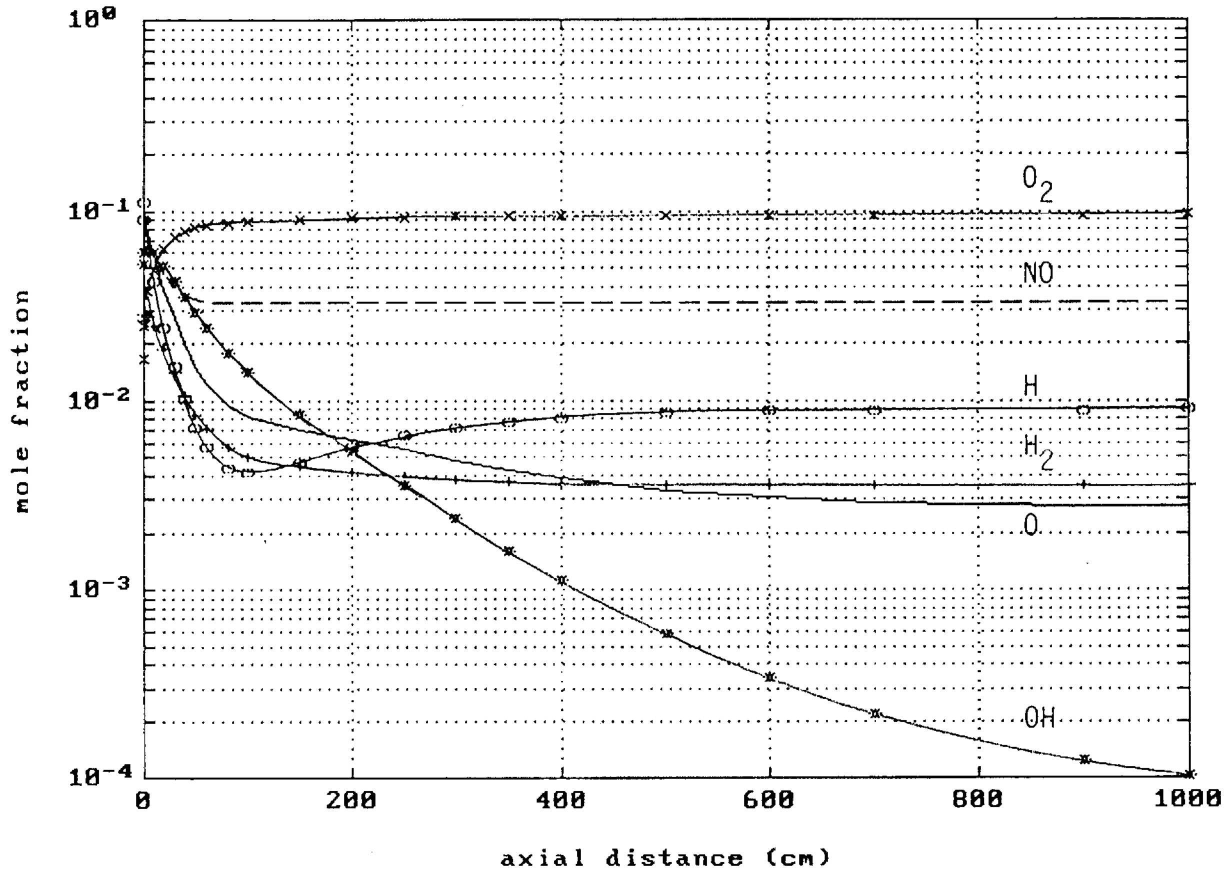
Gas composition during reactive flow through 5^{o} nozzle. Mixing chamber pressure 2554 atm. Air feed

Figure 1b



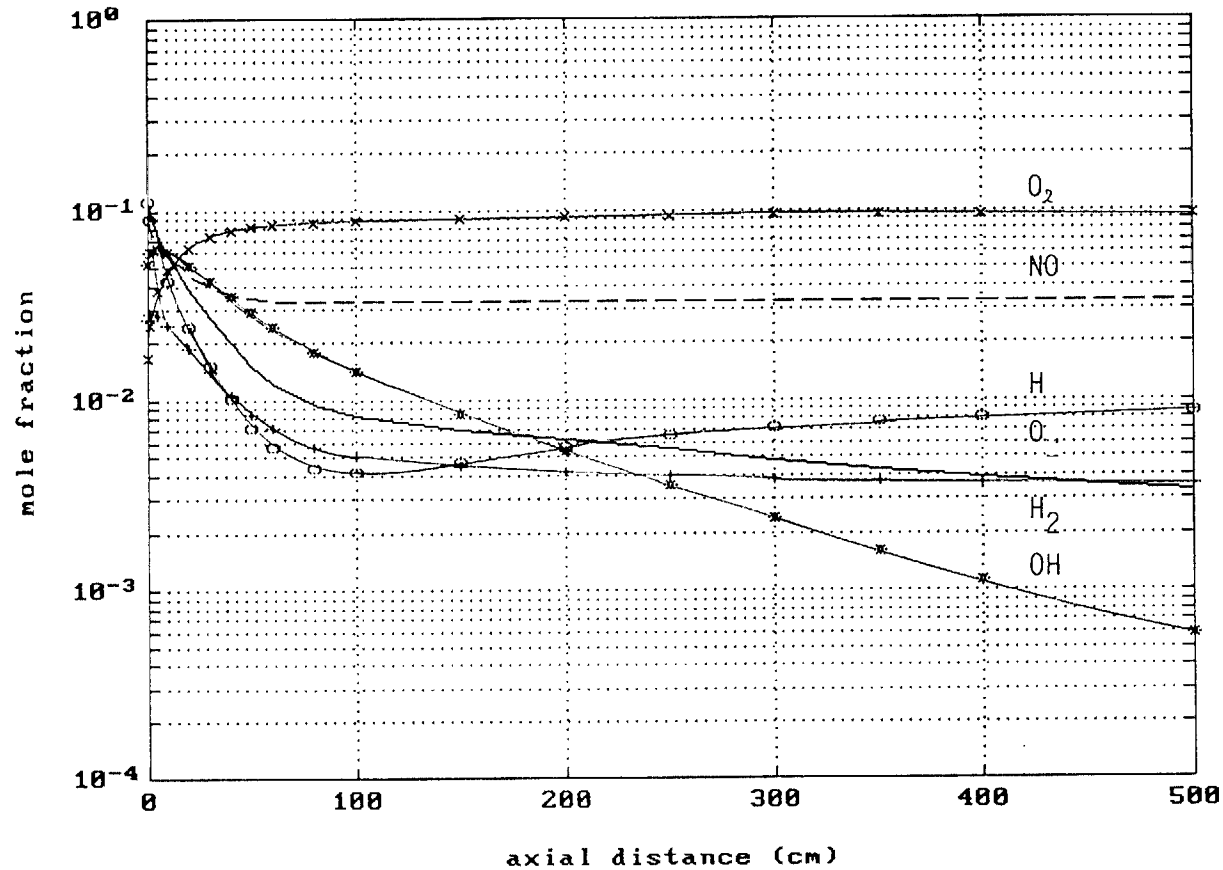
Gas composition during reactive flow through 5^0 nozzle. Mixing chamber pressure 2254 atm.

Figure 2a



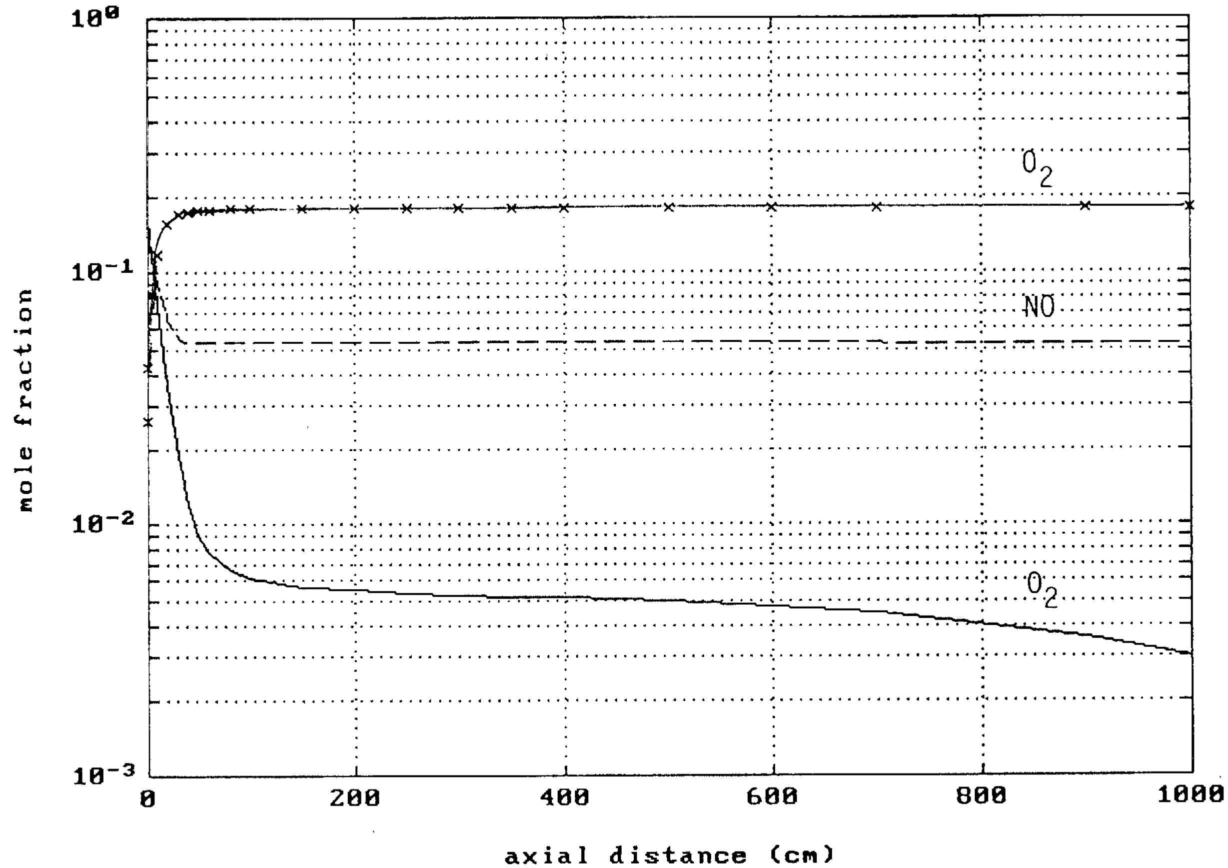
Gas composition during reactive flow through 5^o nozzle. Mixing chamber pressure 2554 atm. Feed is 10% NH_3 in air.

Figure 2b



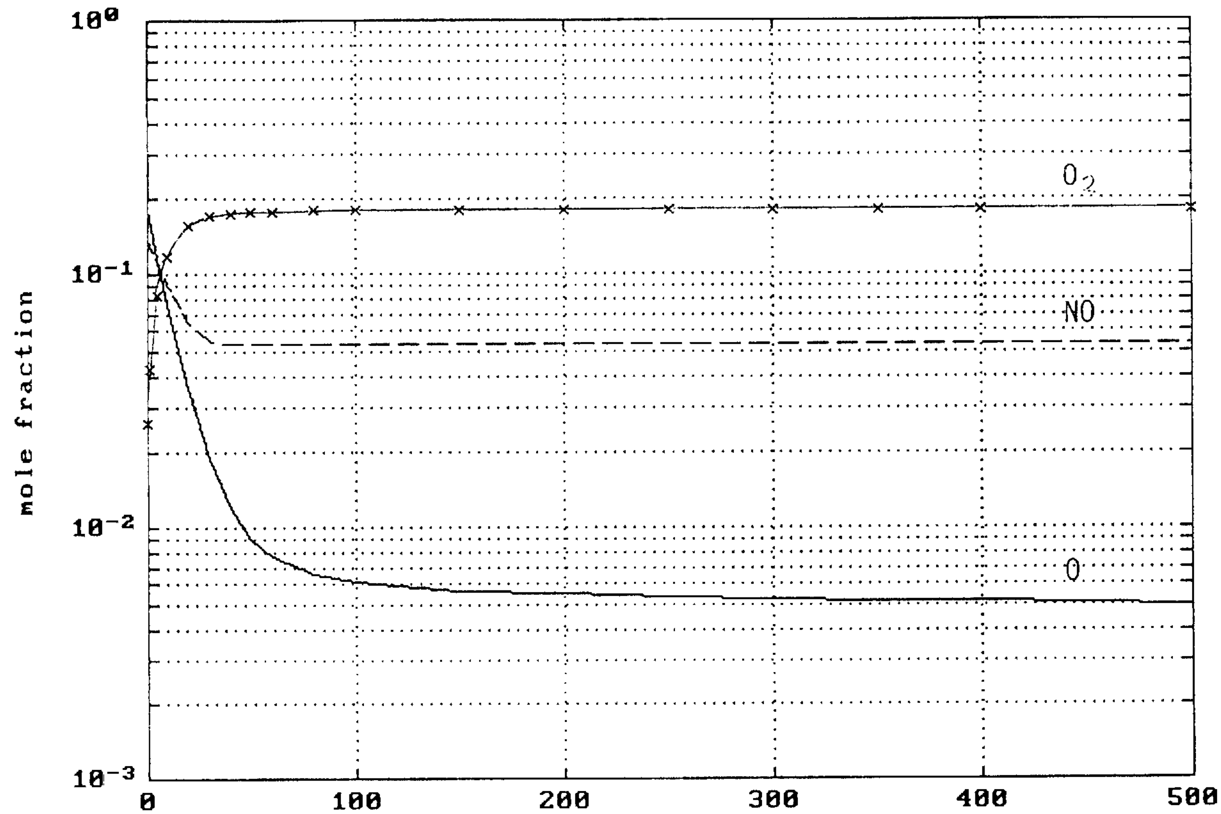
Gas composition during reactive flow through 5^{0} nozzle. Mixing chamber pressure 2554 atm. Feed is 10% NH_3 in air.

Figure 3a



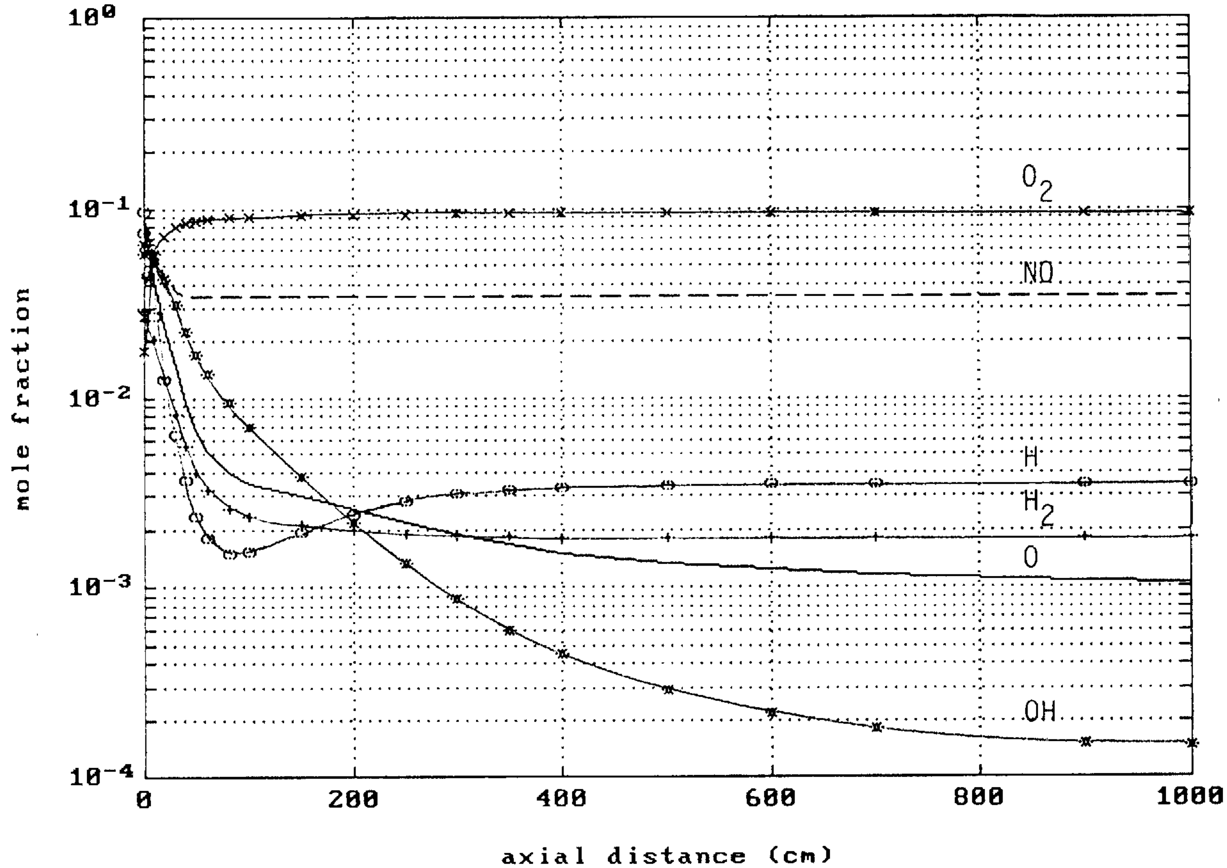
Gas composition during reactive flow through 5^0 nozzle. Mixing chamber pressure 4690 atm. Air feed.

Figure 3b



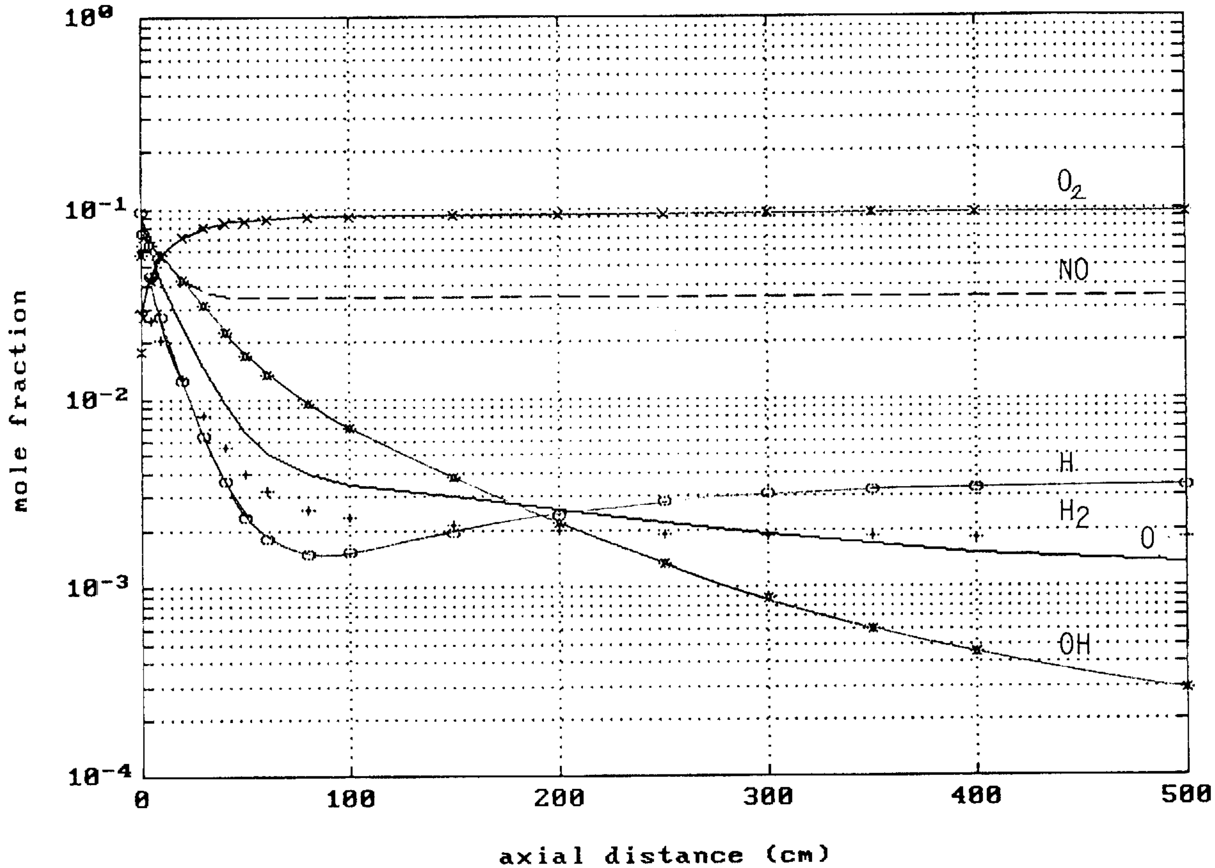
Gas composition during reactive flow through 5^O nozzle. Mixing chamber pressure 4690 atm.

Figure 4a



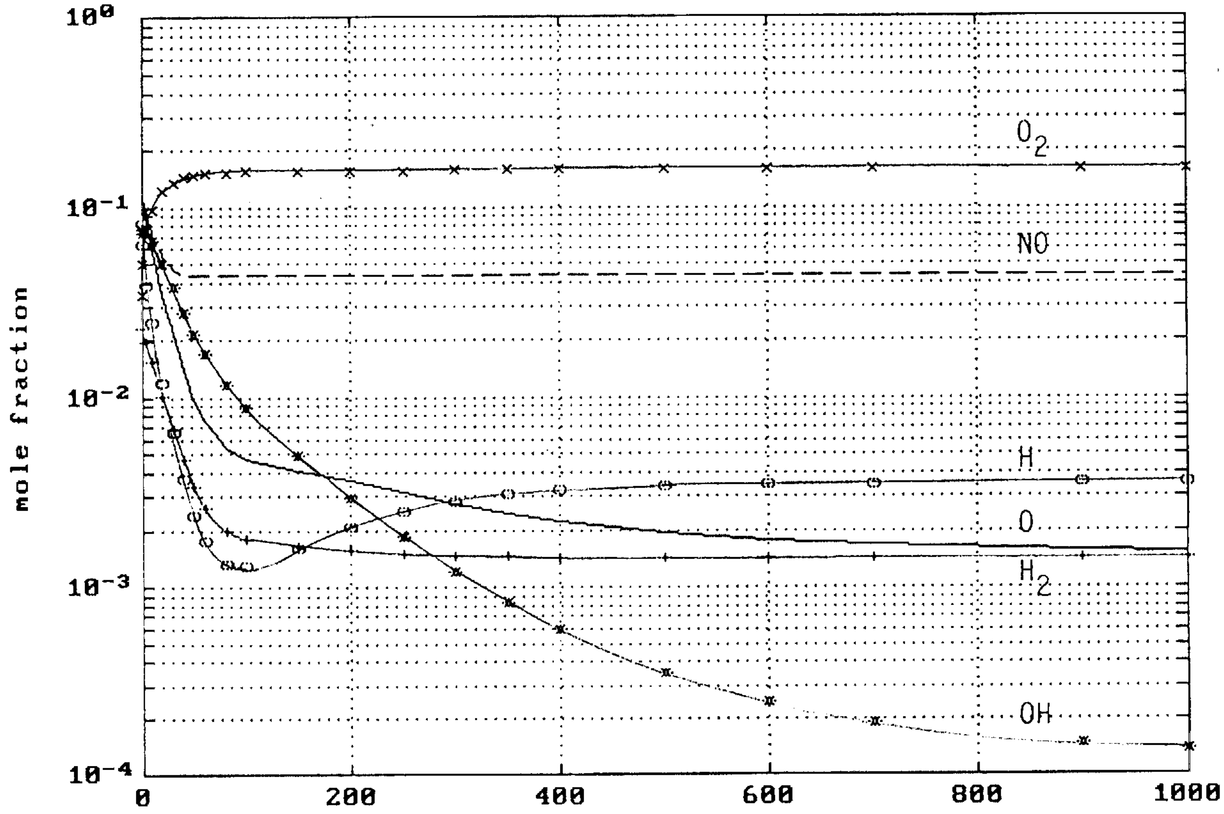
Gas composition during reactive flow through 5^{o} nozzle. Mixing chamber pressure 4690 atm. Feed is 10% NH_3 in air.

Figure 4b



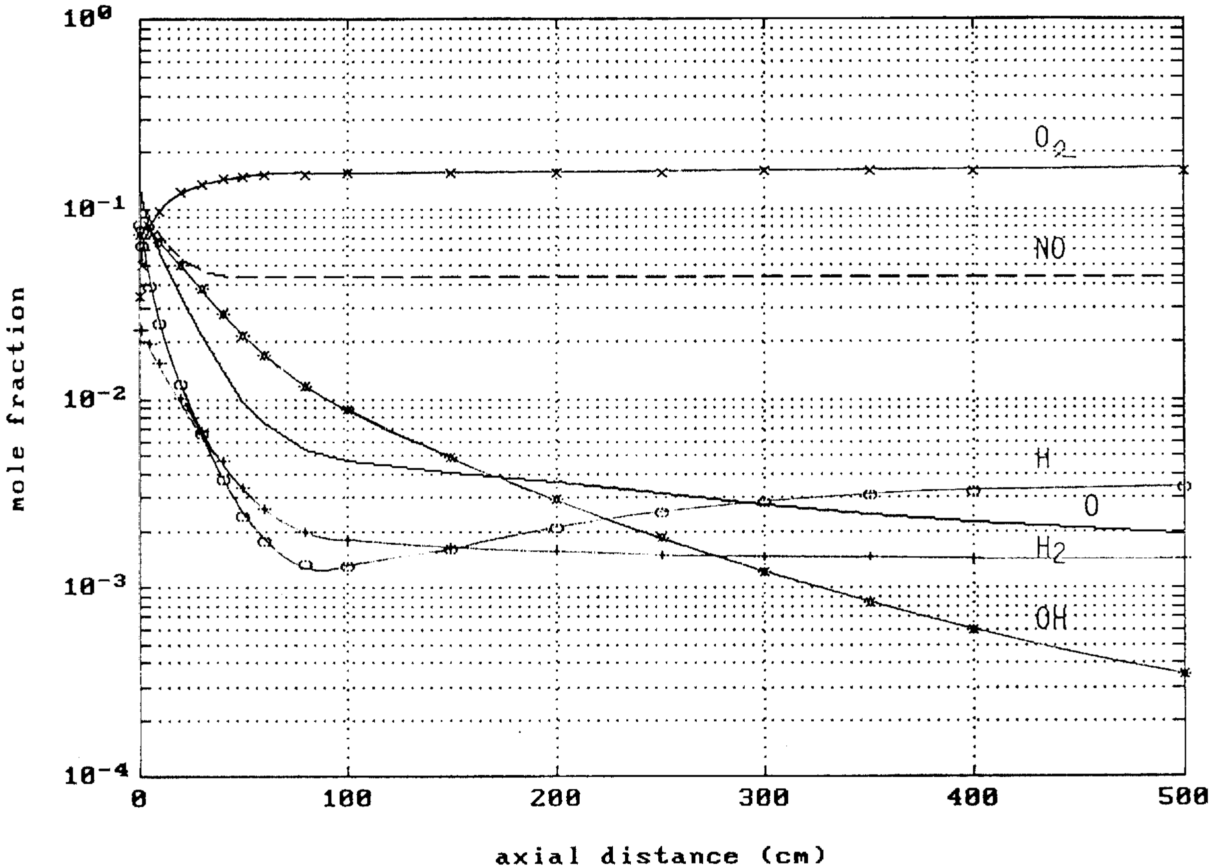
Gas composition during reactive flow through 5° nozzle. Mixing chamber pressure 4690 atm. Feed is 10% NH_3 in air.

Figure 5a



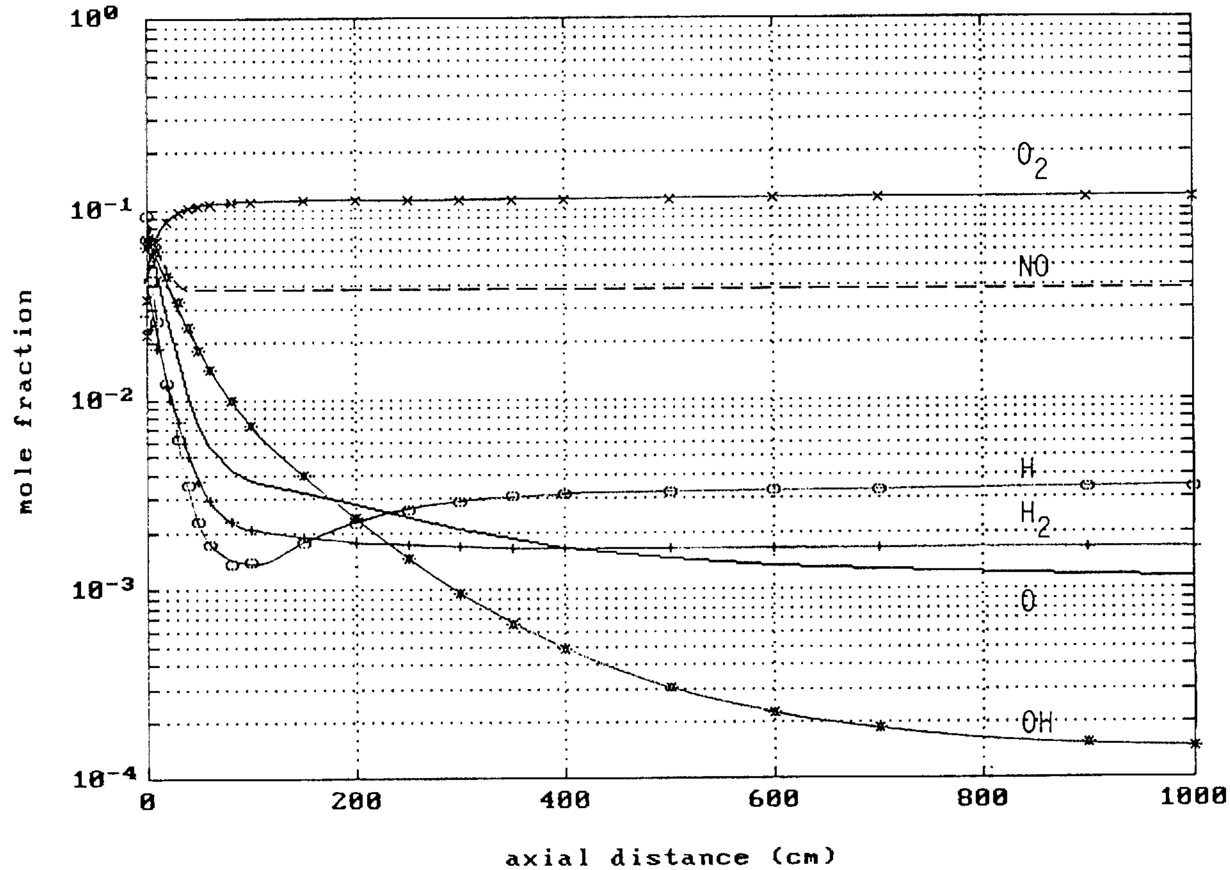
Gas composition during reactive flow through 5^o nozzle. Mixing chamber pressure 4690 atm. Feed is air + H_2O equivalent to H in 10% NH_3.

Figure 5b



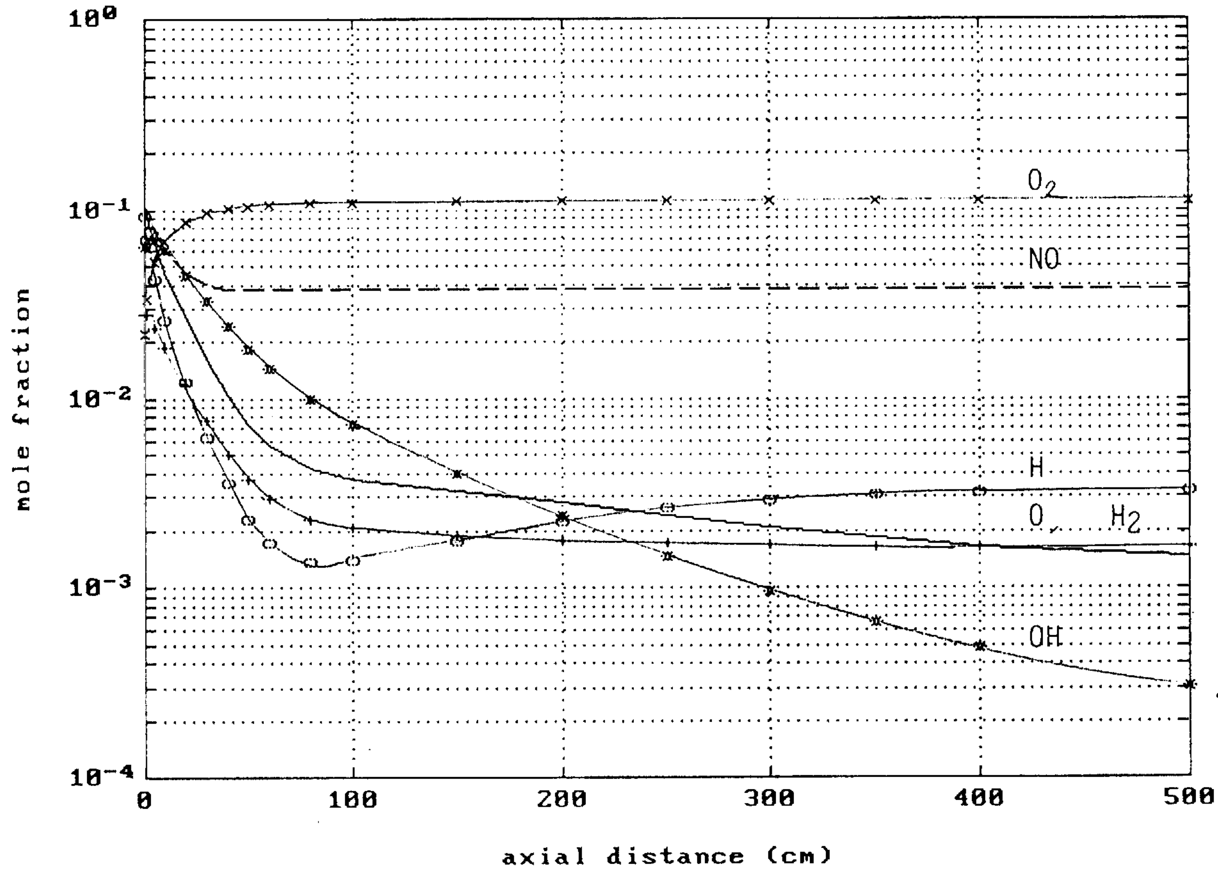
Gas composition during reactive flow through 5^{o} nozzle. Mixing chamber pressure 4690 atm. Feed is air + H_2O equivalent to H in 10% NH_3.

Figure 6a



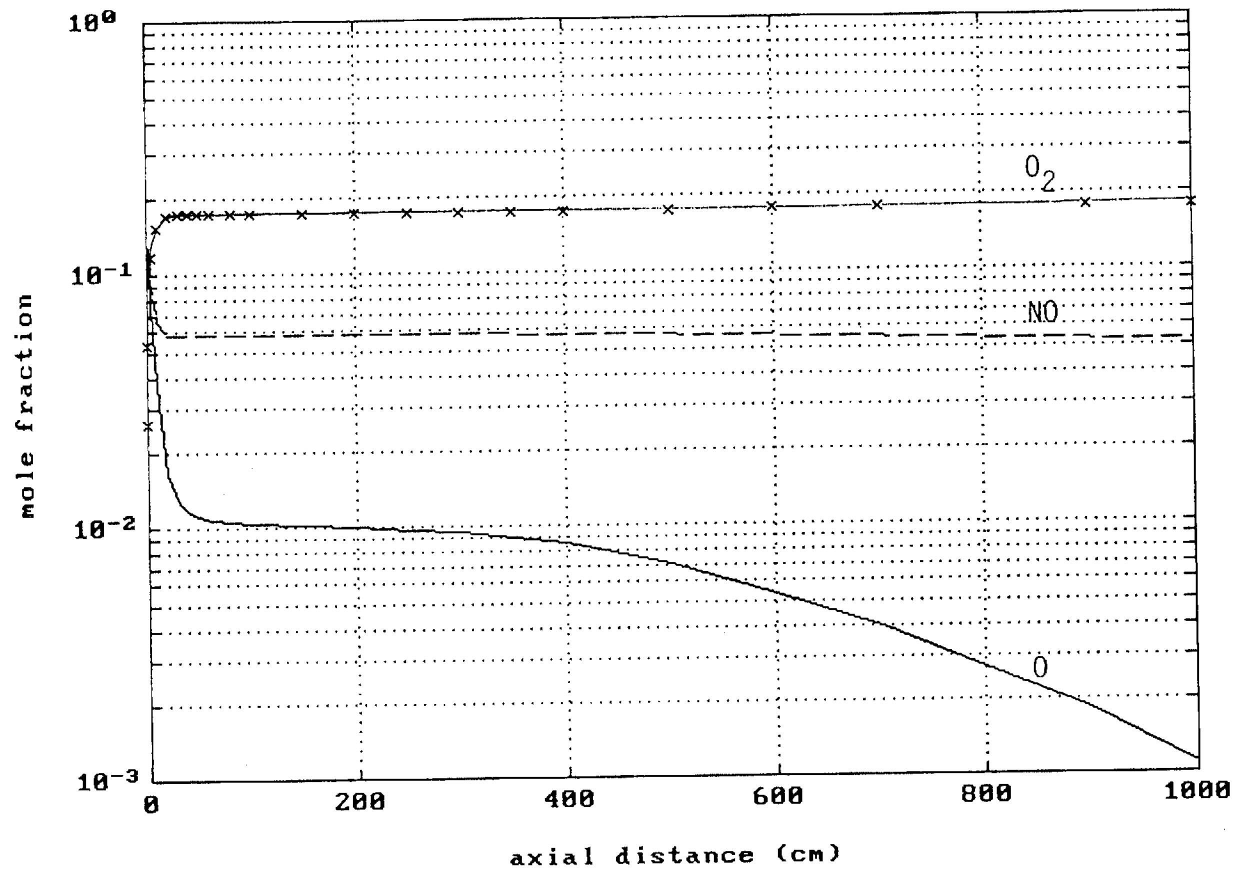
Gas composition during reactive flow through 5^{o} nozzle. Mixing chamber pressure 4690 atm. Some N_2 in air replaced to give 10% NH_3 in the feed.

Figure 6b



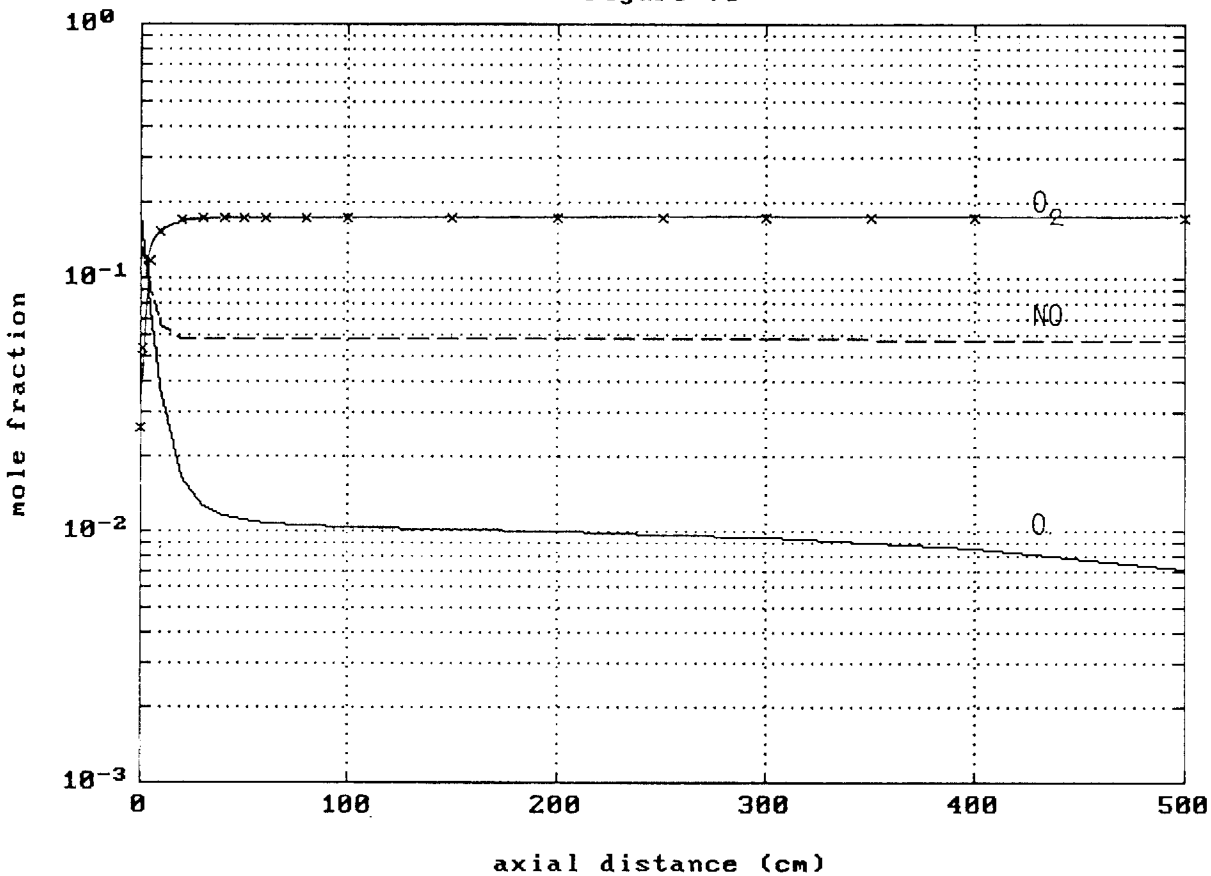
Gas composition during reactive flow through 5^0 nozzle. Mixing chamber pressure 4690 atm. Some N_2 in air replaced to give 10% NH_3 in the feed.

Figure 7a



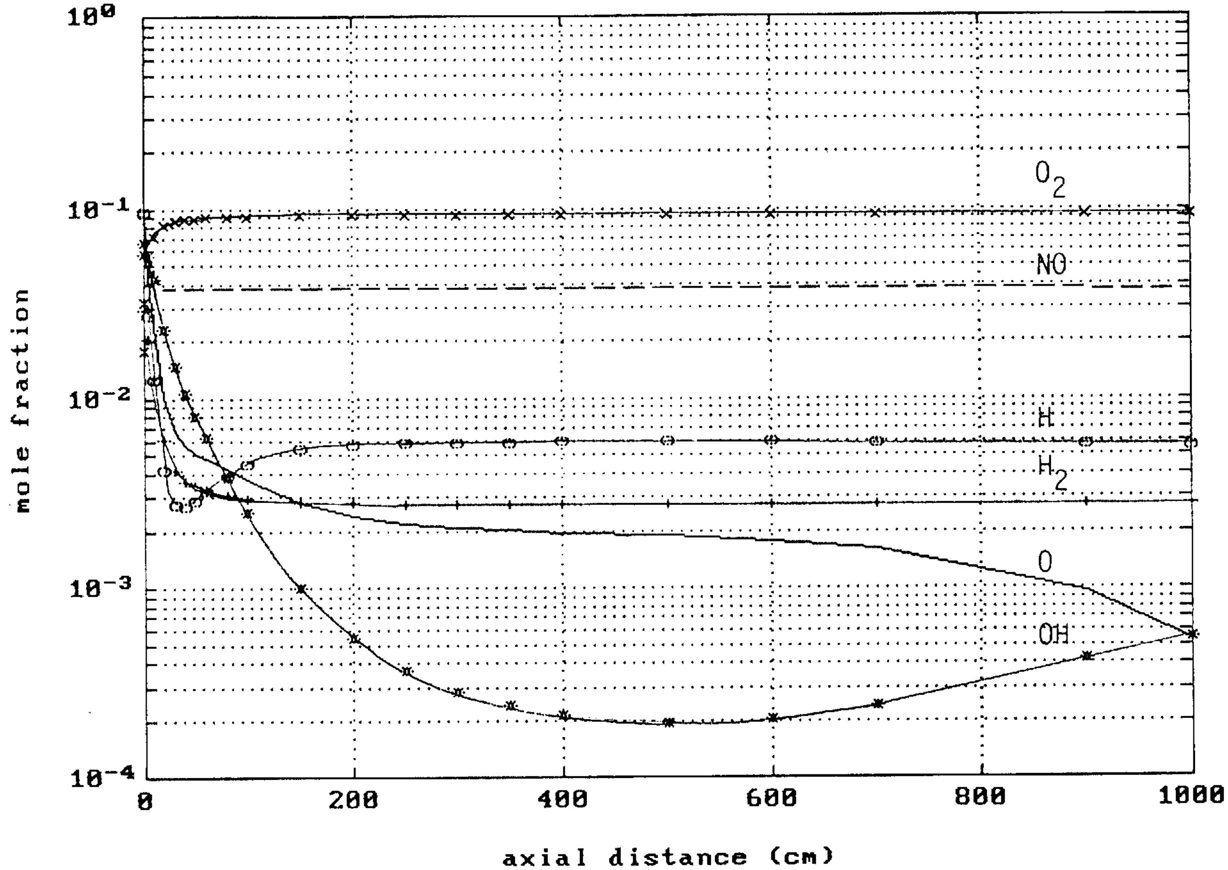
Gas composition during reactive flow through 10^0 nozzle. Mixing chamber pressure 4690 atm. Air feed.

Figure 7b



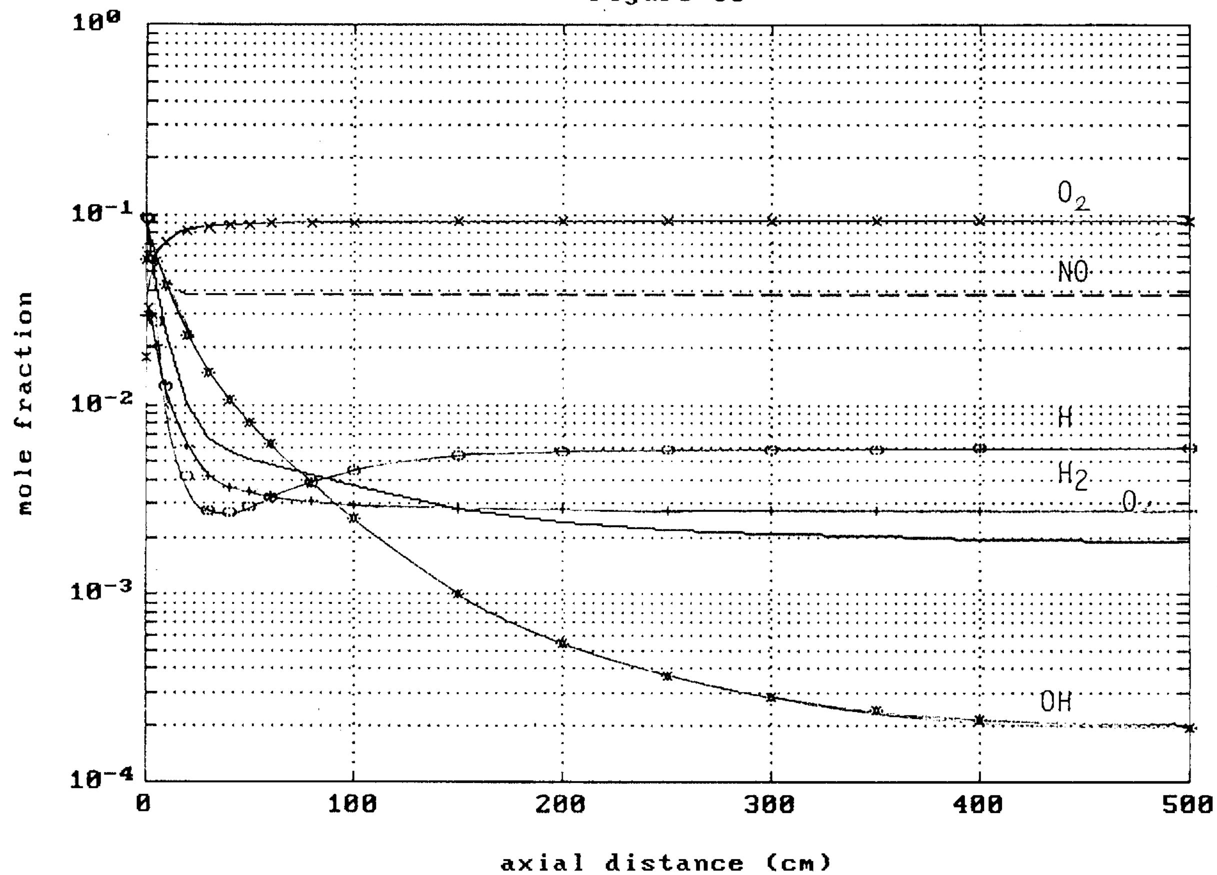
Gas composition during reactive flow through 10° nozzle. Mixing chamber pressure 4690 atm.

Figure 8a



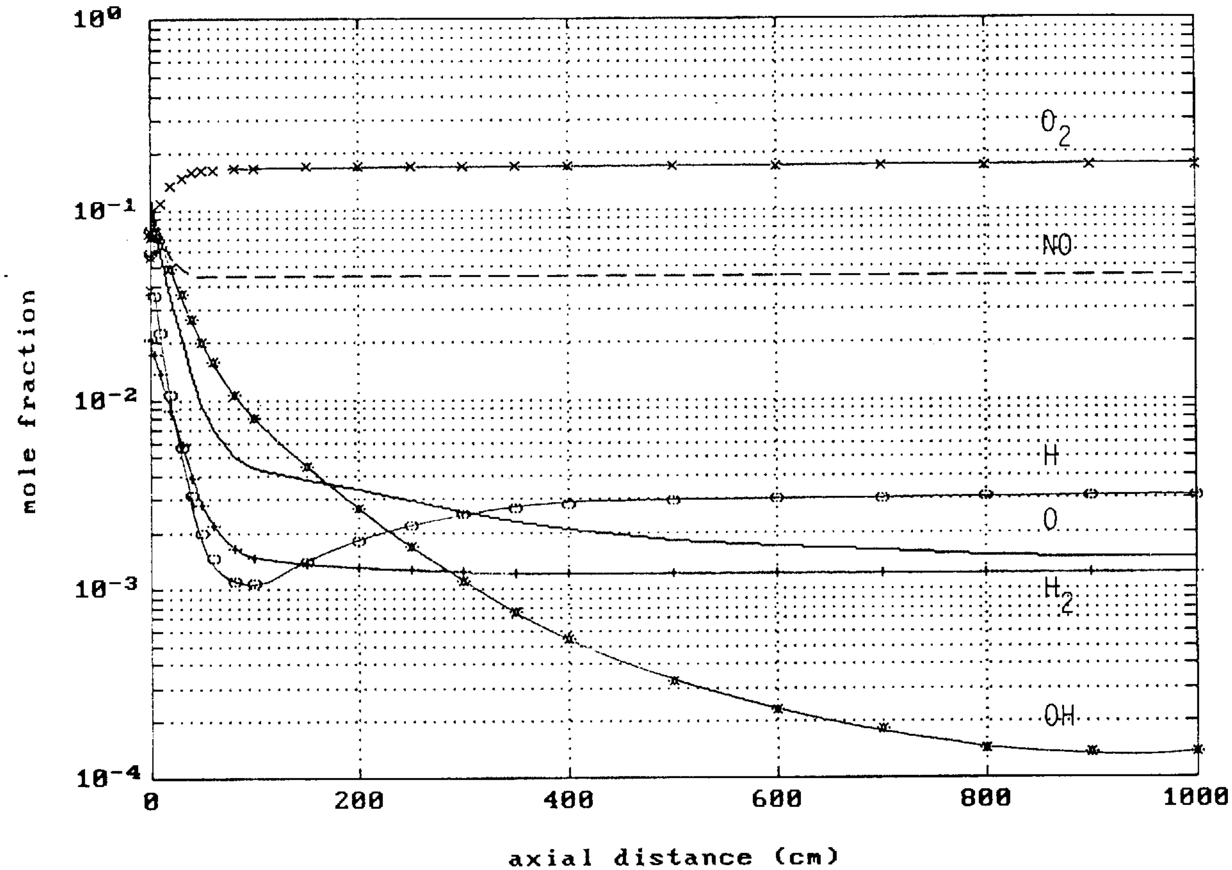
Gas composition during reactive flow through 10^0 nozzle. Mixing chamber pressure 4690 atm. Feed is 10% NH_3 in air.

Figure 8b



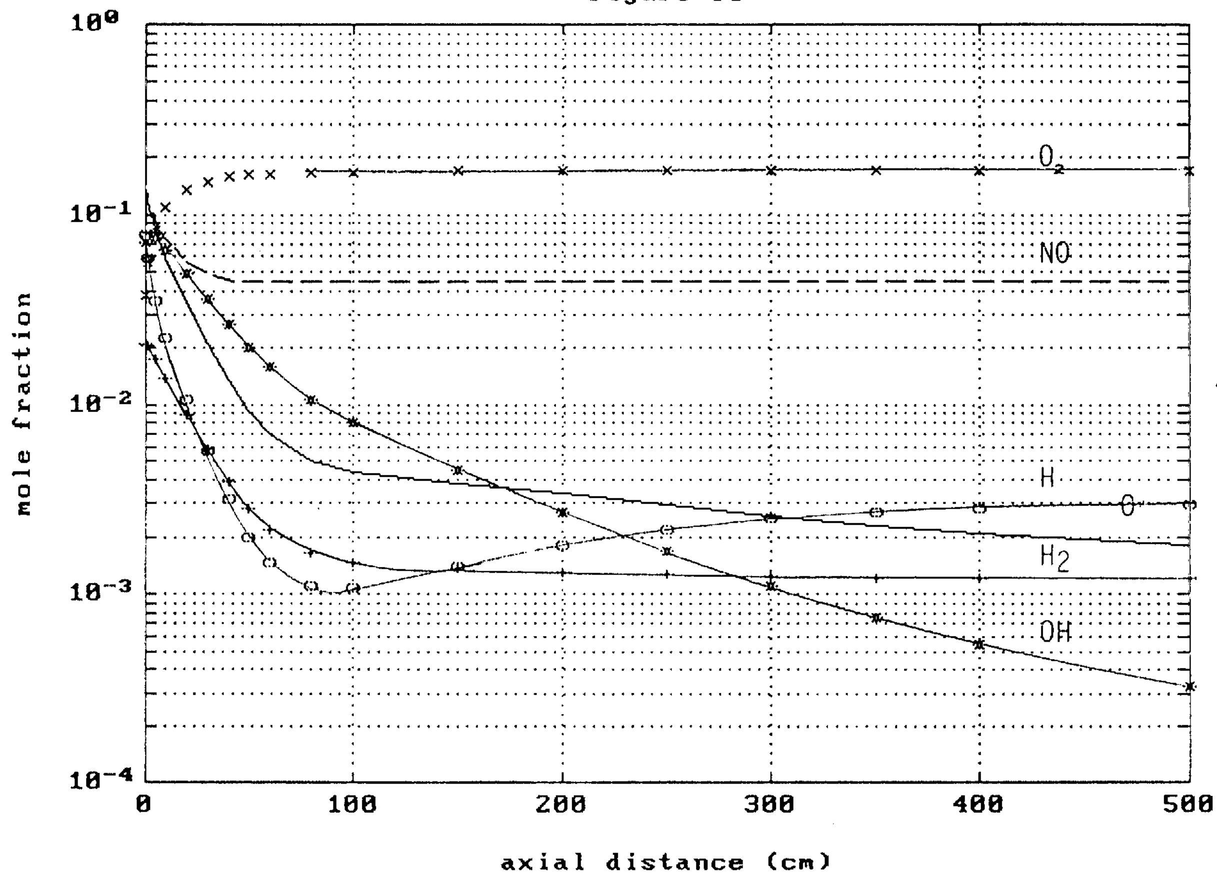
Gas composition during reactive flow through 10^{0} nozzle. Mixing chamber pressure 4690 atm. Feed is 10% NH_3 in air.

Figure 9a



Gas composition during reactive flow through 5^o nozzle. Mixing chamber pressure 4690 atm. Feed is 10% NH_3 in oxygen-enriched air.

Figure 9b



Gas composition during reactive flow through 5^{0} nozzle. Mixing chamber pressure 4690 atm. Feed is 10% NH_3 in oxygen-enriched air.

recombination reactions.

Table 2. Summary of results for reactive nozzle flows for various gas compositions. Ma = Mach Number, y_i = mole fraction of species i.

Gas composition	Air			Air + 10% NH_3			Some N_2 in air replaced by NH_3 to give 10% NH_3	air + H_2O equivalent to H in 10% NH_3
P_0 (atm)	2254	4690	4690	2254	4690	4690	4690	4690
θ (deg .)	5	5	10	5	5	10	5	5
Conditions at 500 cm from nozzle throat								
P (atm)	.0076	.0062	.0009	.0107	.0087	.0012	.0086	.0091
T (K)	636.5	517.6	320.8	863.9	703.4	409.7	714.2	749.1
Ma	10.18	11.37	14.45	8.89	9.91	12.95	9.85	9.68
γ	1.375	1.386	1.399	1.337	1.353	1.384	1.352	1.346
y_O	.0174	.0050	.0070	.0033	.0013	.0019	.0014	.0019
y_{NO}	.0500	.0535	.0570	.0333	.0347	.0381	.0376	.0434
y_{O2}	.1740	.1797	.1753	.0953	.0942	.0932	.1129	.1578
y_H				.0086	.0034	.0059	.0033	.0034
y_{OH}				5.9E-4	2.9E-4	2.0E-4	3.0E-4	3.5E-4
y_{H2}				.0036	.0018	.0028	.0016	.0014
y_{H2O}				.1363	.1416	.1357	.1419	.1385
y_O/y_{O2}	.1000	.0278	.0399	.0346	.0138	.0204	.0124	.0120
y_{NO}/y_{O2}	.2874	.2977	.3252	.3494	.3684	.4088	.3330	.2750

- As expected, a larger nozzle expansion angle freezes the reactions earlier. As a consequence, the mole fractions of O, NO, and H are larger while those of O_2 and H_2 are smaller when the flow is expanded faster. The OH mole fraction is smaller for 10 degree expansion. The most significant changes are observed for the O mole fraction in pure air and H mole fraction in air containing 10% NH_3.
- When column 2 is compared to column 5 it is seen that an original gas mixture containing 10% NH_3 results in a test gas

with significantly lower O and NO mole fractions at the expense of having some H and OH in the test gas. The H mole fraction is over an order of magnitude smaller than that of NO and the OH mole fraction is over an order of magnitude smaller than that of H. Since the O_2 mole fractions are different, to obtain a better comparison, O/O_2 and NO/O_2 ratios are given in rows 15 and 16, respectively. These entries indicate that although the addition of ammonia to air is effective in reducing the O/O_2 ratio, it increases the NO/O_2 ratio due to the presence of a larger number of N atoms.

- Since some air in the feed gas is replaced by NH_3 in the 10% ammonia containing feed, the O_2 mole fraction in the test gas for this case is much lower and the number of N atoms present is much higher than with pure air feed. To obtain a better comparison, the results for a feed gas in which some nitrogen is replaced by ammonia to give 10% NH_3, are given in column 7. Even in this case the O_2 mole fraction is lower than with pure air feed because some oxygen is used to form water. The O/O_2 ratio is lower than that obtained with pure air feed and the NO/O_2 ratio is only slightly higher. There was a significant improvement over the 10% NH_3 feed. The H and H_2 mole fractions are also lower with only insignificant increases in OH and H_2O. Since the OH concentration continues to decrease up to the nozzle exit unlike the other species whose concentrations are frozen after about 500 cm after the nozzle throat, it is expected that the OH mole fraction in the test gas will be lower than the value reported in Table 2.
- To see if the beneficial effect of NH_3 is due to the H_2O formed, the results obtained for a gas feed containing H_2O equivalent to H in the 10% NH_3 feed are included in column 8 of Table 2. These results show that the feed containing H_2O gives the best O/O_2 and NO/O_2 ratios. Even the H_2 and H_2O mole fractions are lower than those in column 6 with only slight increases in H and OH.

Table 3. Summary of results for reactive nozzle flows for various gas compositions. Mixing chamber pressure 4690 atm, nozzle expansion 5 degrees. Ma = Mach number, y_i = mole fraction of species i.

Gas composition	Air	Some N_2 in air replaced by NH_3 to give 10% NH_3 + .08 mol O_2 per mol	Air + H_2O equivalent to H in 10% NH_3
P_0 (atm)	4690	4690	4690
θ (deg .)	5	5	5
Conditions at 500 cm from nozzle throat			
P (atm)	.00618	.00891	.00911
T (K)	517.59	732.05	749.08
Ma	11.37	9.759	9.678
γ	1.3856	1.3483	1.3462
y_O	.004958	.001811	.001924
y_{NO}	.053517	.045193	.043374
y_{O_2}	.179664	.171333	.157830
y_H		.002975	.003408
y_{OH}		.000324	.000354
y_{H_2}		.001204	.001430
y_{H_2O}		.132001	.138533
y_O/y_{O_2}	.027596	.010570	.012190
y_{NO}/y_{O_2}	.297873	.263773	.274815

- To compare the results for feed gas compositions giving similar O_2 mole fractions in the test gas, results were also obtained for a feed gas containing 10% NH_3 and enriched in oxygen to give an O_2 mole fraction similar to that in the test gas obtained with pure air. These results are presented in column 2 of Table 3 and compared with some of the results from Table 2. These results indicate that better O/O_2 and NO/O_2 ratios can be obtained with oxygen enriched air containing 10% NH_3 than air containing water in an amount containing same number of H atoms as in the 10% NH_3 mixture. In addition, the mole fractions of H, OH, H_2, and H_2O are all lower with the 10% NH_3 containing enriched air.

Conclusions

The results shown above indicate that the addition of nitrogen and hydrogen-containing compounds to oxygen-enriched air can improve the O/O_2 and NO/O_2 ratios and can have lower H, OH, H_2, and H_2O mole fractions than with feed gases containing H_2O. It appears that the liquid propellant HAN ($N_2H_4O_4$) may even be a better additive than NH_3 due to its lower N/H ratio and high oxygen content. Other propellants such as HMX, RMX, and HNTO will produce some CO_2 which will reduce the specific heat ratio (thus improving the required stagnation conditions) and increase the rates of recombination reactions in the nozzle. The presence of CO_2 in the test gas may partially counteract the effects of O, H, and OH during combustion tests.

References

1- Rizkalla, O. F.; Chinitz, W.; and Burton, R. : "Mach 10 to 20 Electrothermal Wind Tunnel Feasibility Study and Demonstration", GASL TR 342, Final Report for NAS1-18450, November 1991.

2- McBride, B. J., private communication.

3- Bittker, D. A., private communication.

4- Jachimowski, C. J., "An Analysis of Combustion Studies in Shock Expansion Tunnels and Reflected Shock Tunnels", NASA Technical Paper 3224, 1992.