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PRACTICAL APPLICATION OF COMPUTER PROGRAMS
FOR
SUPERSONIC COMBUSTION

CASE FILE
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Summary

Experimental data obtained by United Aircraft Research Laboratories were interpreted using two supersonic combustion computer programs. Program P1 was an established program based on a conventional boundary layer treatment of the mixing of concentric gas streams and complete combustion chemistry. Program H1 was an untested program based on a modified boundary layer approach which accounted for radial pressure gradients in the flow. Program H1 also incorporated a finite rate chemistry calculation. The objective of the investigation was to compare the experimental data with theoretical predictions of the two programs with special emphasis on the prediction of radial pressure gradients by the H1 program. A test of the H1 program was also desired through comparison with the experimental data and with the P1 program.

The experimental data on specie mass fractions agreed satisfactorily with the theoretical predictions of the P1 program. Agreement improved when the data were adjusted so that the ratio of total oxygen to nitrogen was the same everywhere in the flow field as the overall ratio at the nozzle outlet.

Calculations with the H1 program suggested that the combustion rate observed in the experimental data was not sufficient to produce significant radial pressure gradients. There were indications in the experimental data that the assumptions of complete mixing on a molecular level (on which the finite rate chemistry calculation is based) may not be valid. This fact, together with excessive running time, cast doubt on the usefulness of the finite rate chemistry subroutine for correlating data on supersonic combustion.

Symbols

f_{jH_2}	mass fraction jet hydrogen
k	ratio of specific heat at constant pressure to specific heat at constant volume
m	molecular weight
M	Mach number
P	pressure
r, R	radial distance
T	temperature
u	velocity
x, X	axial distance
$\bar{R}$	universal gas constant
α_i	mass fraction of specie i
α_{CH_2O}	mass fraction of water by combustion
α_{TH_2}	mass fraction total hydrogen including free hydrogen and hydrogen combined as water
Ψ	stream function
ρ	density
μ_e	eddy viscosity

Subscripts

a	free stream conditions
CL	centerline
t	stagnation conditions

Practical Application of Computer Programs for Supersonic Combustion

Introduction

Theoretical studies of supersonic combustion are of considerable interest in connection with combustion chamber design for such vehicles as the hypersonic ramjet. These studies have led to the development of various computer programs for predicting the flow field in supersonic combustion. Early programs of this kind were based on a conventional boundary layer treatment of the mixing and combustion of concentric jets of fuel and air (1). More recently programs have been developed based on a modified boundary layer theory which permits the prediction of lateral pressure gradients produced by the combustion process (2, 3, 4, 5, 6).

Because of a scarcity of data there has been relatively little work done on the comparison of computer predictions with combustion experiments. This report describes work done under contract NAS1-10341 with the object of demonstrating practical application of computer programs in the interpretation of experimental results on supersonic combustion.

Objectives of the Study

Two computer programs were selected for use. The first was prepared by Hopf and Fortune of General Applied Science Laboratories (1). This program is based on the conventional boundary layer equations applied to the mixing and combustion of concentric streams of hydrogen and air. The chemical reaction is handled by assuming complete combustion after

mixing. The partial differential equations that result from the conventional boundary layer equations are of parabolic type, and their solution by the computer is straightforward. This computer program will be referred to hereafter as program P1. Its validity and usefulness in studying turbulent mixing and combustion may be regarded as well established by earlier studies, for example, the work of Anderson, Agnone, and Russin (7).

The second computer program selected for study was written by Groves (5,6) under contracts NAS1-8219 and NAS1-9352. It is based on a modified set of boundary layer equations developed by workers at General Applied Science Laboratories (2). The modifications of the boundary layer theory permit the prediction of radial pressure gradients in the flow field. This is in contrast to program P1 which used the usual boundary layer assumption of constant pressure in the radial direction. Another distinctive feature of the second program is its use of a finite rate chemistry calculation developed by Moretti (8) to describe the combustion reactions. The partial differential equations resulting from the modified boundary layer theory are of a mixed hyperbolic and parabolic type. Their solution by the computer program is described by Groves (5). This second program will be referred to hereafter as the H1 program. It has not been tested against experimental data as yet.

There are two objectives of this study: 1) to use the two programs, P1 and H1, to interpret experimental data on supersonic combustion obtained by United Aircraft Research Laboratories (9). Particular emphasis will be given to the use of the H1 program to predict whether serious pressure gradients will develop in the radial direction as a result of combustion in the mixing zone; (2) to test the H1 program by making various comparisons of results from it with experimental data and with the predictions of well established computer programs.

Interpretation of Experimental Data

The United Aircraft Data

The United Aircraft data were taken in an experimental setup consisting of a coaxial free jet system. The system included a central 2cm diameter hydrogen jet surrounded by a 10cm diameter annular jet containing oxygen, nitrogen, and water vapor. Figure 1 is a schematic diagram of the apparatus. A high temperature was obtained in the annular jet by the process known as vitiation. Hydrogen and air were burned in a vitiation chamber producing high temperature. Various quantities of oxygen were added to the resulting stream to yield the desired composition. The stream was then delivered to a nozzle feeding the annular jet.

The nozzles were designed to produce a Mach 1.46 central jet of hydrogen surrounded by a Mach 1.86 annular jet. Both jets discharged at a pressure of $0.91 \times 10^5 \text{ N/m}^2$ (0.9 atm). Experimental data were taken at stations 0.33cm, 5.1cm, 10.2cm, 17.8cm, 25.4cm, and 35.6cm downstream from the nozzle exit. At each of these stations Pitot pressures and species concentrations (H_2 , H_2O , N_2 , O_2) were measured at various radial positions. For details about the experiments the reader is referred to the report prepared by Cohen and Guile (9).

Experimental data are available for several conditions of the vitiated annular stream. For the purposes of the present contract the data for which the annular jet was adjusted to have an oxygen concentration of approximately 21% were selected for analysis. These data will be referred to henceforward as the high temperature vitiated air data.

Interpretation of the Data Using the P1 Computer Program

Because the parabolic program has a much shorter running time it was decided to test the data against it first. This program assumes complete combustion in its chemistry subroutine so the data could not be compared with the computer results directly. The experimental mass fraction data indicate partial combustion in the mixing zone, and hence must be recalculated on a complete combustion basis before comparison. Furthermore complete combustion implies a greater shifting of streamlines away from the centerline than partial combustion. This means that a comparison of composition data at the same distance from the centerline would not be successful. Instead the experimental data were compared against the computed results at the same value of stream function as done by Anderson, Agnone, and Russin (10).

For axisymmetric geometry the streamline coordinate is defined by:

$$\Psi = \sqrt{2 \int_0^r \rho u r \, dr} \quad (1)$$

To calculate density and velocity it was necessary to know the total temperature at each experimental point. Total temperatures were not measured in the United Aircraft studies for the high temperature vitiated air runs. The values of total temperature calculated by Cohen and Guile (11) in their correlation of the experimental results were therefore used in the calculation of the streamline coordinate. These calculated total temperatures are consistent with the experimentally measured pitot pressures and species concentrations. While their use introduces uncertainty into the calculated values of the stream function, the errors involved should not be serious. The stream function is inversely proportional to the fourth root of the total

temperature. Hence it is not very sensitive to changes in total temperature. This is demonstrated by Table 1 which shows the effect on stream function of 100°K variations.

The Mach number was obtained from the ratio of Pitot pressure to static pressure using the tables given by Shapiro (12). The static temperature was calculated from the total temperature by the relation

$$\frac{T}{T_t} = \frac{1}{1 + \frac{k-1}{2} M^2} \quad (2)$$

with k assumed equal to 1.4. The density and velocity followed directly from the equations:

$$u = M \sqrt{\frac{kRT}{m}} \quad (3)$$

$$\rho = \frac{Pm}{RT} \quad (4)$$

Sufficient information was now available to evaluate the integral in Equation (1). The integral was evaluated numerically from the experimental data using the trapezoidal rule.

The P1 computer program was now run using conditions at the nozzle outlet for the high temperature vitiated air experimental run as input. These starting conditions, as reported by Cohen & Guile (13), are shown in Table 2. The user of the P1 program must also supply a scheme for calculating eddy viscosity at every point in the flow field. For this purpose the Cohen (14) eddy viscosity model was used in the form

$$\mu_e = K \left(\frac{1+n_1}{2} \right)^{0.8} (1-m_1)^b u_{CL} \rho \left[\left(\frac{1+n_1}{1+n} \right) \left(\frac{1+mn}{1+m_1 n_1} \right) \right] \quad (5)$$

The transverse extent of the mixing layer, b , was taken to be the radial distance between the points in the flow where

$$(u-u_a) = 0.95 (u_{CL}-u_a) \quad (6)$$

and

$$(u-u_a) = 0.05 (u_{CL}-u_a) \quad (7)$$

The values of n_1 and m_1 were taken to be 2.69 and 0.6 respectively.

The constant K was adjusted to give good agreement between experimental data and computed results. Its value was 0.0137.

Using these input data the P1 program was run to generate mass fraction vs stream function distributions at axial stations 10.2cm, 17.8cm, 25.4cm, and 35.6cm from the nozzle outlet. The experimental data, recalculated on a complete combustion basis, and the computed results were then compared on plots of mass fraction H_2 , H_2O , N_2 , and O_2 versus stream function. The plots are shown in Figures 2, 3, 4, and 5. The agreement is generally satisfactory although the water mass fraction in the inner jet region is somewhat high at the last two axial stations.

Examination and Adjustment of Composition Data

In an effort to improve agreement between the P1 program and the data an examination of the data for consistency was made. The composition at any point in the flow field results from the mixing of the pure hydrogen from the central jet with the annular stream containing N_2 , O_2 and H_2O . For this reason the ratio of total O_2 (including free O_2 and combined O_2 in the form of H_2O) to N_2 should be the same everywhere in the flow field. This will be true provided that mixing by the movement of turbulent eddies predominates over mixing by molecular diffusion and providing that the composition of the annular stream at the nozzle outlet is uniform.

Calculation of the total O_2 to N_2 ratio revealed variations from

point to point in the flow field at all axial stations including the nozzle outlet. These variations may be due to errors in the sampling procedure and the gas chromatographic analysis which yielded the composition data. On the other hand they may result from insufficient mixing upstream of the nozzle outlet causing a non-uniform concentration distribution in the annular stream at the nozzle outlet. The available data are not sufficient to decide which explanation of the variable O_2 to N_2 ratio is correct. It was decided to explore the consequences of assuming a uniform flow field at the nozzle outlet and adjusting the data to give a constant ratio of total O_2 to N_2 . Table 3 shows the overall composition of the annular stream as reported by Cohen and Guile (13) along with the total O_2 to N_2 ratio. A computer program was written to adjust the data to this ratio of O_2 to N_2 at every point.

There are three possibilities for adjusting the data to the proper O_2 to N_2 ratio:

Method A: Assume N_2 and O_2 correct, adjust H_2O

Method B: Assume N_2 and H_2O correct, adjust O_2

Method C: Assume O_2 and H_2O correct, adjust N_2 .

The data were recalculated by these three methods. A priori method A seemed most likely to be correct because accurate analysis for H_2O is probably most difficult. As a check on the three methods total H_2 flow was calculated at the axial stations 10.2, 17.8, 25.4, and 35.6cm from the nozzle exit. The calculation of total H_2 flow is discussed in Appendix I.

Table 4 shows the total H_2 flow based on the three correction methods. All three methods result in a H_2 flow significantly less than the metered flow of 0.051 kg/sec. This same discrepancy was observed

by Cohen and Guile (15) in the treatment of other data from the same experimental equipment. The total H_2 flow stays more nearly constant from station to station for method A. For this reason and because of the greater probability of error in the water analysis, Method A was chosen for treatment of the data.

Table 5 shows uncorrected mass fraction data and mass fraction data adjusted by method A at each axial station. The stream function is also shown. A study of the data revealed that the adjusted values do not scatter as badly as the raw data. Figure 6 illustrates this for the nitrogen mass fractions at the 17.8cm axial station.

Figures 7, 8, 9, and 10 compare the data, adjusted by Method A to a constant O_2/N_2 ratio, with the predictions of the P1 program. The agreement is somewhat more satisfactory than for the uncorrected data. This may simply reflect better consistency of the corrected data with the uniform annular stream composition used as input to the P1 program.

Interpretation of the Data Using the H1 Computer Program

Having demonstrated agreement of the experimental data with the P1 program, attention was now turned to the hyperbolic H1 program. The H1 program was run with the same input data used previously (Table 2). The Cohen eddy viscosity equation with the same numerical parameters used with the P1 program was used in this run. Because the H1 program includes finite rate chemistry it was necessary to add to the data of Table 2 information about the mass fractions of the free radical species, H, O, and OH. In the first run these were set equal to zero. Under these conditions the H1 program ran successfully, but ignition did not occur.

It was suggested by Cohen and Guile (16) in their discussion of the experimental data that the hot vitiated air stream contains increased amounts of free radicals produced during the vitiation process. Accordingly the free radical concentrations (H , O , OH) for the input data were increased to the levels suggested by Cohen and Guile as shown in Table 6. The H1 program started successfully under these conditions and ignition did occur. However, the calculated pressure and temperature soon rose rapidly resulting in a decrease in Mach number to the subsonic range. At this point the H1 program failed. The H1 program involves application of the method of characteristics to the hyperbolic part of the equations describing the flow. When the Mach number falls below 1.0, the method of characteristics fails.

The H1 computer program ran successfully to an axial position 8.02cm from the nozzle outlet before failing. The predicted mass fractions of H_2 , O_2 , H_2O , and N_2 were therefore compared with the experimental data (adjusted by Method A, not completely reacted) at the 10.2cm axial position. Figure 11 shows that agreement is satisfactory. Only slightly less satisfactory agreement was found between the raw data and the calculated results. This indicates the general validity of the H1 program in the region ahead of the high heat release.

The main reason for applying the H1 program to the experimental data was to see if the program predicts large radial pressure gradients as a result of rapid release of heat by the chemical reaction in the mixing zone. The results indicate that, given the rate of heat release predicted by the finite rate chemistry calculation, the radial pressure gradients are indeed severe. This conclusion still leaves the question whether the heat release rate predicted by the finite rate chemistry subroutine agrees with the heat release rate observed experimentally. This question will be examined in the following section.

Introduction of the Partial Combustion Chemistry Subroutine

Since the high rate of heat release predicted by the finite rate chemistry routine appeared to be causing trouble, alternative approaches to the combustion chemistry were sought. In a turbulent flow field mixing occurs by the movement of slugs or eddies of material from one place in the flow field to another. Thus the mixing zone in the United Aircraft experiments may consist of slugs of H_2 distributed among slugs of O_2 rich material but not necessarily mixed on a molecular level. The finite rate chemistry subroutine, which assumes complete mixing on a molecular level, may not provide an accurate description of the combustion process in a real turbulent field.

A partial combustion chemistry subroutine was therefore developed. The H1 program carries out a stepwise calculation of the turbulent flow field in the axial direction. For each axial step a characteristics calculation first computes pressures for each radial position at the next axial point. Next a calculation of radial mixing of mass, energy, and momentum is made. Finally the finite rate chemistry subroutine computes the extent of reaction at the new axial position.

The partial combustion chemistry routine allows a fixed percentage of the limiting reactant to be consumed by the combustion process at each radial position. For example, if at a certain point in the flow field oxygen is present in excess then hydrogen is the limiting reactant. The chemistry routine reacts a fixed percentage of the hydrogen and leaves the rest unreacted. At another position the hydrogen might be present in excess, and the given percentage of oxygen would be reacted. This procedure is repeated for every radial position at each axial step. The fixed percentage reaction is supplied to the computer program with

the rest of the starting data. Though this percentage may be small, after a hundred axial steps a considerable amount of reaction has occurred.

The H1 program modified in this way was run with the high temperature vitiated air input data (Table 2) used previously. With percentage reaction in a given step limited to less than 4%, the program ran successfully. A rapid increase in temperature occurred in the mixing zone. The temperature increase was accompanied by an increase in pressure but this pressure increase soon changed to an oscillation. The Mach number remained in the supersonic range, and the calculation could be continued as far as desired in the axial direction.

Calculated pressure distributions, radial and axial, are shown in Figures 12 and 13 based on one per cent reaction in each axial step. It can be seen that the combustion process does not produce large pressure gradients when the burning rate is limited in this way.

Partial combustion with a fixed percentage reaction in each axial step is only a crude way to describe the actual reaction process. A better approximation would be the use of a variable percentage reaction, higher in the hot parts of the flow field, lower in the cool parts. The calculations based on a fixed percentage reaction were not expected to predict correctly the details of radial distribution of chemical species present. However, the partial combustion chemistry does provide a way for the user of the H1 program to control the rate of heat release by the combustion process.

A method was now sought to compare heat release rate for the experimental data with heat release rate in the partial combustion chemistry

computer runs. A good measure of the total heat release up to a given point in the flow field is the mass fraction of water formed by combustion up to that point. Accordingly this mass fraction was now calculated for the experimental data and for the computer run.

The calculation is made somewhat more difficult by the fact that the water present at any point in the flow field comes from two sources - combustion of hydrogen and oxygen and mixing of water fed from the nozzle with the annular stream. The water from the annular stream can be calculated, however, by using nitrogen from the annular stream as a tracer. The overall water to nitrogen mass ratio in this stream at the nozzle outlet is 0.254. This ratio is not changed by the turbulent mixing process. Thus, assuming a uniform composition for the annular stream at the nozzle outlet, the mass fraction of water from the annular stream at any point in the flow field is 0.254 times the mass fraction nitrogen at that point. The mass fraction water by combustion is then readily obtained by deducting the water from the annular stream from the total mass fraction of water at any point.

$$\alpha_{\text{CH}_2\text{O}} = \alpha_{\text{H}_2\text{O}} - 0.254 \alpha_{\text{N}_2}$$

Figure 14 compares the water by combustion derived from the raw experimental data with the water by combustion predicted by the computer at axial stations 10.2, 17.8, and 25.4cm from the nozzle outlet. At each axial station the experimental water formed by combustion is less than or equal to the calculated combustion water. While not conclusive this certainly suggests that the rate of water formation and hence the rate of heat release by combustion was greater in the computer calculations than in the experimental run.

The experimental values shown in Figure 14 are based on the assumption that the water to nitrogen mass ratio in the annular stream is equal to 0.254 uniformly throughout the flow field at the nozzle outlet. If the experimental data at the 0.33cm axial station are correct the water to nitrogen ratio is somewhat higher than 0.254 in the neighborhood of the hydrogen jet. Assuming negligible combustion at $x = 0.33\text{cm}$ this would imply somewhat lower peaks in the experimental combustion water data than shown on Figure 14. This in turn would reinforce our conclusion that the experimental water by combustion is less than that observed in the computer runs.

Water by combustion was also calculated from the adjusted experimental data of Table 5. The calculated values are considerably lower than the points shown in Figure 14. In fact if the adjusted data are correct, there was little combustion occurring in the experimental run. The UAC investigators observed a flame but there was a "flickering" effect (17) which suggests marginal combustion. There does not appear to be sufficient information to decide whether the raw or adjusted data are correct. In either case our conclusion that there was more rapid combustion in the computer run than in the experiment holds.

We are thus led to the answer to one of the prime questions raised by this investigation: Is the experimental heat release rate sufficiently large to produce significant radial pressure gradients? The heat release rate in the computer run did not produce severe radial pressure gradients. Since the heat release rate in the experimental run appears to be even less we conclude that significant radial pressure gradients do not develop there.

It is interesting to inquire how complete the combustion process

was in the computer run plotted on Figure 14. Figure 15 compares the combustion water for total combustion in this computer run with the combustion water actually calculated based on 1% reaction per step. It can be seen that significant combustion occurred in the computer run.

If the experimental points of Figure 14 were plotted on Figure 15 they would form a curve of the same general shape but with a peak lower and to the left of the partial combustion curve. Evidently by using a lower percentage combustion per step (perhaps 0.5% instead of 1%) it would be possible to get a reasonable match of computer predictions with experimental results. It is interesting that such a crude model of the chemistry offers the possibility of a rough reproduction of experimental results.

Testing of the H1 Computer Program

The H1 computer program is a new program which has not been adequately tested against experimental data and otherwise. One of the objectives under the present contract was to perform general tests of the validity of the H1 program. Several of these tests will now be discussed.

Comparison of Results with GASL Program

The first trial of the H1 program was a comparison on a test case with a similar program prepared by General Applied Science Laboratories. The input data are shown in Table 7. The purpose of the run was to test the characteristics and mixing parts of the program so the chemistry subroutine was eliminated.

Figure 16 shows how centerline pressure varied with axial position for this test case. Mixing of the hot and cold streams gave rise to a pressure increase, but this increase never exceeded a few per cent. Furthermore the pressure variations appear to be damping out. The predictions of the H1 program agreed in this respect with the GASL program (18). Although exact quantitative agreement with the GASL program was not achieved the differences can probably be attributed to differences in radial and axial step-size in the numerical method. The results show that the characteristics and mixing parts of H1 are stable and converge to reasonable answers.

Nozzle Calculation by H1 Program

Calculation of the flow through a nozzle described by Shoemaker (19)

was used as a test of the characteristics portion of the H1 program. Pure hydrogen was used as the flowing fluid; the chemistry subroutines were bypassed; and the parabolic mixing equations were nullified by setting eddy viscosity equal to zero.

The nozzle was a Mach 2.22 nozzle whose contour was fitted by means of three polynomials. The contour is shown in Table 8. Conditions at the nozzle inlet are shown in Table 9. Some difficulty was experienced in obtaining a good polynomial fit of the nozzle contour. Although the fitted curve could be made to conform to the given points on the nozzle contour, the fit tended to be "wavy".

The program ran successfully and predicted conditions at the nozzle outlet as shown in Table 10. Conditions at the nozzle outlet check in a general way with expected results. The nozzle design calls for a Mach number of 2.22 at the outlet. The Mach numbers in Table 10 are in the right range. The predicted results indicate a significant radial gradient in pressure. This may be the result of failure to achieve an exact polynomial fit of the nozzle contour.

Comparison of the H1 Program with the P1 Program

To test the mixing portion of the H1 program a comparison with the P1 program was used. The two programs were run with starting data for the United Aircraft high temperature vitiated air experiments. The chemistry portion of the H1 program was bypassed. The chemistry calculation in the P1 program was eliminated by using pure nitrogen in the hot outer jet to mix with pure hydrogen in the inner jet. For both programs a constant eddy viscosity of $6 \times 10^{-4} \frac{\text{slugs}}{\text{ft sec.}}$ was used.

The programs were run out to an axial position of 0.6 ft where a comparison was made. Figure 17 shows plots of static temperature and hydrogen mass fraction versus radial position for the two programs. Figure 18 shows the axial distribution of hydrogen mass fraction as predicted by the two programs. The agreement is good indicating again the validity of the mixing and characteristics portion of the H1 program.

Discussion of the Finite Rate Chemistry Subroutine

This study casts significant doubt on the usefulness of the finite rate chemistry subroutine for interpreting experimental data on supersonic combustion. One difficulty is the long running time of this subroutine. Two hours of IBM 360-65 central processing unit time is a reasonable estimate for computing a 30cm long combustion chamber using the starting conditions of the United Aircraft experimental run discussed in this report. This compares to about 10 minutes of CPU time for the same calculation using the H1 program with the finite rate chemistry bypassed. Efforts to shorten the running time by reducing the number of chemical reactions included in the finite rate chemistry routine did not appear rewarding and were abandoned.

Another serious difficulty is that the heat release rate predicted by the finite rate chemistry calculation appears to be considerably greater than observed in the experiments examined in this investigation. The finite rate chemistry routine assumes complete

mixing of the flowing fluid on a molecular level. In a turbulent flow field this degree of mixing is not immediately attained. In the experiment studied here the field probably consists of eddies or slugs of hydrogen distributed among eddies of oxygen rich material but not mixed with them on a molecular level. The combustion rate is therefore limited not by finite rate chemistry but by the rate of molecular interdiffusion between adjacent hydrogen rich and oxygen rich eddies. This explains the slower rate of heat release suggested by the experimental data. It would seem desirable to develop a chemistry calculation based on this interdiffusion process (20) rather than the complete microscopic mixing model used in the H1 program. It may be that the reaction rate is so fast that the combustion process is completely controlled by the interdiffusion rate. In this case the complex free radical scheme of chemical reactions, which requires so much computer time, would not need to be considered.

Conclusions

1. There was satisfactory agreement between the raw experimental mass fraction data and the theoretical predictions of the P1 program. The agreement improved when the raw data were adjusted so that the nitrogen to oxygen ratio was the same everywhere in the flow field.
2. Calculations with the H1 computer program suggest that the heat release rate observed in the experimental data is not sufficient to produce significant radial pressure gradients under the experimental conditions (free jet).
3. Tests of the characteristics and mixing portions of the H1 program indicate that the program is stable and predicts results in general agreement with experimental data and the P1 program.
4. Tests of the finite rate chemistry portion of the H1 program indicate that the running time is excessive and suggest that the assumption of complete mixing of chemical species on a molecular level is in disagreement with experimental data.
5. Efforts should be made to develop a chemistry subroutine that reflects the controlling effect of interdiffusion of adjacent turbulent eddies on the combustion rate.

Appendix I

Calculation of Total Flow Rate of Hydrogen from Central Jet

At any point in the flow field the hydrogen present comes from two sources: the central jet and the water present in the annular stream. As a check on the experimental data the total flow of hydrogen originating from the central jet was calculated from the experimental data for each axial station. This total flow should remain the same at each axial station and should equal the jet hydrogen flow calculated from conditions at the nozzle outlet.

The total jet hydrogen flow was calculated by evaluating the integral

$$2\pi \int_0^R f_{jH_2} \rho u r dr \quad (I-1)$$

at each axial station. The first step in the computation was the determination of f_{jH_2} , the mass fraction of central jet hydrogen at a given point in the flow field. The mass fraction total hydrogen (including free hydrogen and hydrogen in the form of water) was easily obtained:

$$\alpha_{TH_2} = \alpha_{H_2} + \frac{1}{9} \alpha_{H_2O} \quad (I-2)$$

The mass fraction of hydrogen from the annular stream was calculated by using nitrogen as a tracer for water from the annular stream. The overall mass ratio of water to nitrogen in the annular stream was 0.254. This ratio should remain the same everywhere in the flow field provided that mixing by turbulent transport predominates over

molecular diffusion and assuming that the annular stream is uniform at the nozzle outlet. The mass fraction of central jet hydrogen was computed by deducting the hydrogen equivalent to the annular stream water from the total hydrogen mass fraction

$$f_{jH_2} = \alpha_{H_2} + \frac{1}{9} \alpha_{H_2O} - \left(\frac{0.254}{9}\right) \alpha_{N_2} \quad (I-3)$$

Density and velocity were computed as described on page 5 in connection with calculation of the stream function. The integral of equation I-1 was evaluated by the trapezoidal rule.

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Table 1

Effect of Variations in Total Temperature
on
Stream Function

<u>X = 17.8cm</u>		$\Psi - (\text{kg/sec})^{1/2}$	
R, cm	Total Temperature Decreased 100°K	Total Temperature as Used	Total Temperature Increased 100°K
0.0	0.00	0.00	0.00
0.3175	0.03775	0.03625	0.03502
0.635	0.07176	0.06936	0.06734
1.016	0.1094	0.1065	0.1041
1.27	0.1374	0.1344	0.1317
1.397	0.1539	0.1507	0.1480
1.524	0.1749	0.1716	0.1687
1.778	0.2287	0.2250	0.2217
1.895	0.2555	0.2516	0.2481
2.022	0.2841	0.2800	0.2762
2.212	0.3266	0.3220	0.3178
2.53	0.3984	0.3928	0.3875
2.911	0.4823	0.4753	0.4688
3.165	0.5363	0.5285	0.5212
3.292	0.5629	0.5546	0.5470
3.419	0.5891	0.5805	0.5724
3.673	0.6407	0.6312	0.6224
3.810	0.6681	0.6582	0.6490

Table 2

Starting Data for Computer Programs: High Temperature Vitiated Air

<u>Jet:</u>		<u>Annular Stream:</u>	
radius	1cm		
α_{H_2}	1.0	α_{H_2}	0.0
α_{H_2O}	0.0	α_{H_2O}	0.15
α_{N_2}	0.0	α_{N_2}	0.59
α_{O_2}	0.0	α_{O_2}	0.26
Temperature	276°K	Temperature	1031°K
Pressure	$0.91 \times 10^5 \text{ N/m}^2$ (0.9 atm)	Pressure	$0.91 \times 10^5 \text{ N/m}^2$ (0.9 atm)
Velocity	1877 m/sec.	Velocity	1240 m/sec.

Table 3

Conditions at Nozzle Outlet for High Temperature
Vitiated Air Experiment

<u>Jet:</u>	Radius	1cm
	α_{H_2}	1.0
	Mach Number	1.46
	Pressure	$0.91 \times 10^5 \text{ N/m}^2$ (0.9 atm)

Annular Stream:

	α_{H_2}	0.0
	α_{H_2O}	0.15
	α_{N_2}	0.59
	α_{O_2}	0.26
	Mach Number	1.86
	Pressure	$0.91 \times 10^5 \text{ N/m}^2$ (0.9 atm)
	Mass Ratio of total oxygen to nitrogen	0.666

Table 4

Total Jet Hydrogen Flow Rate

	<u>Hydrogen Flow, Kg/sec.</u>		
	X = 10.2cm	X = 17.8cm	X = 25.4cm
Raw Data	0.044	0.036	0.034
Method A	0.044	0.034	0.034
Method B	0.045	0.038	0.035
Method C	0.038	0.032	0.030
			X = 35.6cm
			0.029
			0.035
			0.031
			0.027

Hydrogen Flow at Nozzle Outlet: 0.051 Kg/sec.

Method A: N₂ and O₂ assumed correct, H₂O adjustedMethod B: N₂ and H₂O assumed correct, O₂ adjustedMethod C: O₂ and H₂O assumed correct, N₂ adjusted

Table 5

Experimental Mass Fraction Data for High Temperature Vitiated Air

$$X = 0.33\text{cm}$$

$\dot{V}(\text{kg/sec})^{1/2}$	R, cm	α_{H_2}		$\alpha_{\text{H}_2\text{O}}$		α_{N_2}		α_{O_2}	
		Raw Data	Corrected	Raw Data	Corrected	Raw Data	Corrected	Raw Data	Corrected
0.0386	0.3175	1.00	1.00	0.0	0.0	0.0	0.0	0.0	0.0
0.0750	0.635	1.00	1.00	0.0	0.0	0.0	0.0	0.0	0.0
0.1134	0.997	1.00	1.00	0.0	0.0	0.0	0.0	0.0	0.0
0.1154	1.016	1.00	1.00	0.0	0.0	0.0	0.0	0.0	0.0
0.1272	1.143	0.648	0.720	0.1151	0.0179	0.1506	0.1671	0.086	0.096
0.1517	1.27	0.0	0.0	0.246	0.1183	0.506	0.592	0.248	0.290
0.1872	1.397	0.0	0.0	0.1775	0.1225	0.555	0.592	0.268	0.286
0.220	1.524	0.0	0.0	0.1581	0.1357	0.576	0.591	0.266	0.273
0.277	1.778	0.0	0.0	0.1702	0.1423	0.571	0.590	0.258	0.267
0.328	2.032	0.0	0.0	0.1712	0.1608	0.582	0.589	0.247	0.250
0.358	2.184	0.0	0.0	0.1604	0.1417	0.578	0.590	0.262	0.268
0.363	2.212	0.0	0.0	0.1466	0.1752	0.609	0.588	0.245	0.236
0.426	2.53	0.0	0.0	0.1414	0.1569	0.600	0.590	0.258	0.254
0.500	2.911	0.0	0.0	0.1304	0.1536	0.606	0.590	0.264	0.257
0.525	3.038	0.0	0.0	0.1276	0.0892	0.569	0.594	0.303	0.317
0.552	3.175	0.0	0.0	0.1332	0.1408	0.596	0.591	0.271	0.268
0.574	3.291	0.0	0.0	0.1316	0.1233	0.586	0.592	0.282	0.285
0.676	3.810	0.0	0.0	0.1734	0.0963	0.543	0.594	0.284	0.310
0.831	4.572	0.0	0.0	0.1019	0.1400	0.617	0.591	0.282	0.269

Table 5 (Continued)

Experimental Mass Fraction Data for High Temperature Vitiated Air

$$X = 10.2 \text{ cm}$$

$\dot{V}, (\text{kg/sec})^{1/2}$	R, cm	α_{H_2}		$\alpha_{\text{H}_2\text{O}}$		α_{N_2}		α_{O_2}	
		Raw Data	Corrected	Raw Data	Corrected	Raw Data	Corrected	Raw Data	Corrected
0.01505	0.127	1.00	1.00	0.0	0.0	0.0	0.0	0.0	0.0
0.0576	0.508	1.00	1.00	0.0	0.0	0.0	0.0	0.0	0.0
0.0742	0.660	1.00	1.00	0.0	0.0	0.0	0.0	0.0	0.0
0.0853	0.762	0.769	0.857	0.092	0.0	0.0767	0.0855	0.0626	0.0570
0.1117	1.016	0.444	0.543	0.251	0.083	0.219	0.268	0.0861	0.1054
0.1398	1.270	0.1420	0.1614	0.235	0.1303	0.435	0.494	0.1882	0.214
0.1871	1.524	0.0	0.0	0.223	0.1825	0.558	0.588	0.218	0.230
0.246	1.778	0.0	0.0	0.1793	0.1454	0.567	0.590	0.254	0.264
0.301	2.02	0.0	0.0	0.1595	0.1718	0.597	0.588	0.243	0.240
0.304	2.03	0.0	0.0	0.1720	0.1677	0.586	0.589	0.242	0.243
0.385	2.40	0.0	0.0	0.1539	0.1539	0.590	0.590	0.256	0.256
0.412	2.53	0.0	0.0	0.1397	0.1416	0.592	0.590	0.268	0.268
0.438	2.66	0.0	0.0	0.1471	0.1571	0.596	0.590	0.256	0.253
0.491	2.91	0.0	0.0	0.1458	0.1558	0.597	0.590	0.258	0.255
0.543	3.16	0.0	0.0	0.1394	0.1151	0.576	0.592	0.284	0.292
0.594	3.42	0.0	0.0	0.1543	0.1465	0.585	0.590	0.261	0.263
0.644	3.67	0.0	0.0	0.1503	0.1636	0.598	0.589	0.251	0.247
0.671	3.81	0.0	0.0	0.1708	0.0720	0.532	0.595	0.297	0.333
0.794	4.44	0.0	0.0	0.1605	0.0907	0.548	0.594	0.291	0.315

Table 5 (Continued)

Experimental Mass Fraction Data for High Temperature Vitiated Air

 $X = 17.8\text{cm}$

$\psi, (\text{kg/sec})^{1/2}$	R, cm	α_{H_2}		$\alpha_{\text{H}_2\text{O}}$		α_{N_2}		α_{O_2}	
		Raw Data	Corrected	Raw Data	Corrected	Raw Data	Corrected	Raw Data	Corrected
0.00	0.0	0.818	0.840	0.0372	0.0102	0.0924	0.0950	0.0528	0.0543
0.0362	0.3175	0.774	0.792	0.0424	0.0205	0.1209	0.1237	0.0628	0.0642
0.0694	0.635	0.645	0.659	0.0842	0.0645	0.1963	0.200	0.0748	0.0764
0.1065	1.016	0.359	0.362	0.1539	0.1471	0.370	0.373	0.1172	0.1181
0.1344	1.27	0.1880	0.210	0.230	0.1410	0.417	0.465	0.1655	0.1846
0.1507	1.397	0.1275	0.1388	0.232	0.1639	0.465	0.506	0.1760	0.1915
0.1716	1.524	0.0568	0.0706	0.290	0.1170	0.442	0.550	0.211	0.262
0.225	1.778	0.0	0.0	0.212	0.1784	0.564	0.588	0.244	0.234
0.252	1.895	0.0	0.0	0.1560	0.0505	0.530	0.597	0.314	0.353
0.280	2.02	0.0	0.0	0.1670	0.201	0.612	0.586	0.221	0.212
0.322	2.21	0.0	0.0	0.1369	0.1527	0.601	0.590	0.262	0.257
0.393	2.53	0.0	0.0	0.1398	0.1453	0.594	0.590	0.266	0.264
0.475	2.91	0.0	0.0	0.1377	0.1558	0.602	0.590	0.260	0.254
0.528	3.16	0.0	0.0	0.1338	0.1273	0.587	0.592	0.279	0.281
0.555	3.29	0.0	0.0	0.1362	0.1514	0.600	0.590	0.263	0.259
0.580	3.42	0.0	0.0	0.1557	0.1237	0.570	0.592	0.274	0.284
	3.67	0.0	0.0	0.1529	0.1395	0.581	0.591	0.266	0.270
	3.81	0.0	0.0	0.210	0.1031	0.522	0.593	0.267	0.304
	4.44	0.0	0.0	0.1393	0.1032	0.569	0.593	0.291	0.304

Table 5. (Continued)

Experimental Mass Fraction Data for High Temperature Vitiated Air

$$X \approx 25.4\text{cm}$$

$\psi, (\text{kg/sec})^{1/2}$	R, cm	α_{H_2}		$\alpha_{\text{H}_2\text{O}}$		α_{N_2}		α_{O_2}	
		Raw Data	Corrected	Raw Data	Corrected	Raw Data	Corrected	Raw Data	Corrected
0.0141	0.127	0.597	0.649	0.1011	0.0223	0.1920	0.209	0.1097	0.1194
0.0353	0.3175	0.542	0.562	0.0983	0.0652	0.249	0.258	0.1102	0.1143
0.0701	0.635	0.466	0.498	0.1456	0.0851	0.276	0.295	0.1131	0.1211
0.1120	1.016	0.275	0.302	0.1908	0.1127	0.375	0.411	0.1588	0.1742
0.1435	1.270	0.1480	0.1688	0.243	0.1367	0.429	0.490	0.1796	0.205
0.1807	1.524	0.0890	0.0924	0.221	0.1920	0.512	0.532	0.1772	0.1839
0.227	1.778	0.0303	0.0287	0.1519	0.1984	0.602	0.570	0.215	0.2034
0.316	2.21	0.0	0.0	0.1926	0.1558	0.564	0.590	0.244	0.255
0.384	2.53	0.0	0.0	0.1218	0.1413	0.604	0.590	0.274	0.268
0.520	3.16	0.0	0.0	0.1275	0.1390	0.599	0.591	0.274	0.270
0.646	3.81	0.0	0.0	0.1563	0.0982	0.555	0.593	0.288	0.308
0.752	4.44	0.0	0.0	0.1323	0.1227	0.585	0.592	0.282	0.285
	5.08	0.0	0.0	0.0922	0.1417	0.625	0.590	0.283	0.268

Table 5 (Continued)

Experimental Mass Fraction Data for High Temperature Vitiated Air

$$X = 35.6\text{cm}$$

$\Psi, (\text{kg/sec})^{1/2}$	R, cm	α_{H_2}		$\alpha_{\text{H}_2\text{O}}$		α_{N_2}		α_{O_2}	
		Raw Data	Corrected	Raw Data	Corrected	Raw Data	Corrected	Raw Data	Corrected
0.01422	0.127	0.467	0.528	0.1551	0.0454	0.248	0.280	0.1296	0.1465
0.0371	0.330	0.366	0.379	0.1488	0.1198	0.353	0.365	0.1311	0.1367
0.0697	0.635	0.361	0.413	0.1773	0.0584	0.304	0.348	0.1574	0.1802
0.1141	1.016	0.1879	0.1942	0.1989	0.1720	0.457	0.472	0.1566	0.1618
0.1456	1.270	0.1723	0.1742	0.203	0.1940	0.477	0.482	0.1477	0.1494
0.1813	1.524	0.0848	0.990	0.237	0.1099	0.457	0.533	0.221	0.258
0.202	1.651	0.0466	0.0482	0.1936	0.1651	0.541	0.560	0.219	0.227
0.224	1.778	0.0452	0.0447	0.1472	0.1559	0.569	0.563	0.239	0.236
0.272	2.02	0.0	0.0	0.1528	0.1884	0.613	0.587	0.234	0.224
0.312	2.21	0.0	0.0	0.1195	0.250	0.685	0.583	0.1954	0.1663
0.377	2.52	0.0	0.0	0.0918	0.1664	0.642	0.589	0.266	0.245
0.505	3.16	0.0	0.0	0.0945	0.1764	0.647	0.588	0.259	0.235
0.601	3.67	0.0	0.0	0.1026	0.1429	0.618	0.590	0.279	0.266
0.624	3.81	0.0	0.0	0.227	0.222	0.581	0.585	0.1916	0.1929
0.721	4.44	0.0	0.0	0.1149	0.1804	0.635	0.588	0.250	0.232
	5.08	0.0	0.0	0.1068	0.210	0.662	0.586	0.231	0.204

Table 6

Mass Fraction Free Radicals in
Starting Data for H1 Program

α_H	2.99×10^{-8}
α_{OH}	5.42×10^{-4}
α_O	1.874×10^{-5}

Table 7

Starting Data for Comparison of H1 Program
with GASL Program

	<u>Central Jet</u>	<u>Annular Stream</u>
Mach Number	2	3
Velocity	1269 m/sec.	1041 m/sec.
Temperature	1000°K	300°K
Pressure	$1.013 \times 10^5 \text{ N/m}^2$ (1 atm)	$1.013 \times 10^5 \text{ N/m}^2$ (1 atm)
Gas	air	air

radius of central jet = 2.5cm

Eddy viscosity = $2.49 \times 10^{-2} \frac{\text{N-sec}}{\text{m}^2}$ (constant)

Table 8

Nozzle Contour for Test of H1 Program

x axial distance cm	r radial distance cm
0.0	0.3535
0.0354	0.3570
0.0707	0.3623
0.1414	0.3747
0.2828	0.3995
0.4242	0.4242
0.5656	0.4461
0.707	0.4638
0.9191	0.4850
1.1312	0.4977
1.3433	0.5027
1.5625	0.5041

Polynomial fit: $x < 0.03\text{cm}$:

$$r = 0.3535 + 2.48 \times 10^{-5} x + 0.193x^2 + 67.5x^3$$

 $0.03\text{cm} \leq x < 1.1\text{cm}$:

$$r = 0.350 + 0.196(x-0.03) - 0.0428(x-0.03)^2 - 0.0129(x-0.03)^3$$

 $1.1\text{cm} \leq x < 1.36\text{cm}$:

$$r = 0.497 + 0.05501(x-1.1) - 0.133(x-1.1)^2 + 0.105(x-1.1)^3$$

 $x \geq 1.36\text{cm}$

$$r = 0.504$$

Table 9

Conditions at Nozzle Inlet for Test H1 Program

Mach Number	1.1
Temperature	434.8°R
Pressure	$1.61 \times 10^6 \text{ N/m}^2$ (15.9 atm)
Velocity	1296 m/sec.
Gas	hydrogen

Table 10

Calculated Results at Nozzle Outlet: H1 Program

<u>x = 1.56cm:</u>		$P_{CL} = 2.56 \times 10^5 \text{ N/m}^2 (2.52 \text{ atm})$	
r, cm	P/P _{CL}	u, m/sec	Mach Number
0.0	1.0	2130	2.36
0.0394	1.001	2130	2.36
0.0789	1.003	2125	2.35
0.1180	1.010	2125	2.35
0.1580	1.018	2120	2.35
0.1970	1.029	2120	2.34
0.237	1.048	2115	2.33
0.276	1.072	2110	2.32
0.315	1.107	2100	2.30
0.355	1.141	2090	2.28
0.394	1.175	2080	2.26
0.434	1.200	2078	2.24
0.473	1.206	2074	2.24
0.504	1.205	2070	2.23

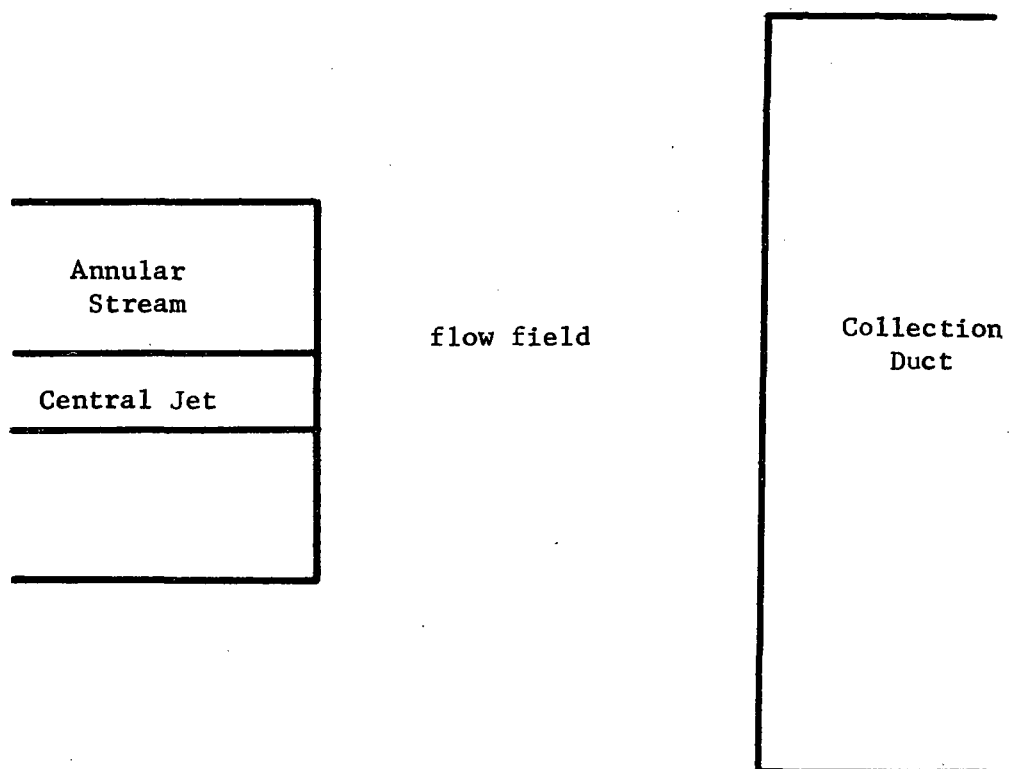


Figure 1
Schematic Diagram
of
United Aircraft Experimental Setup

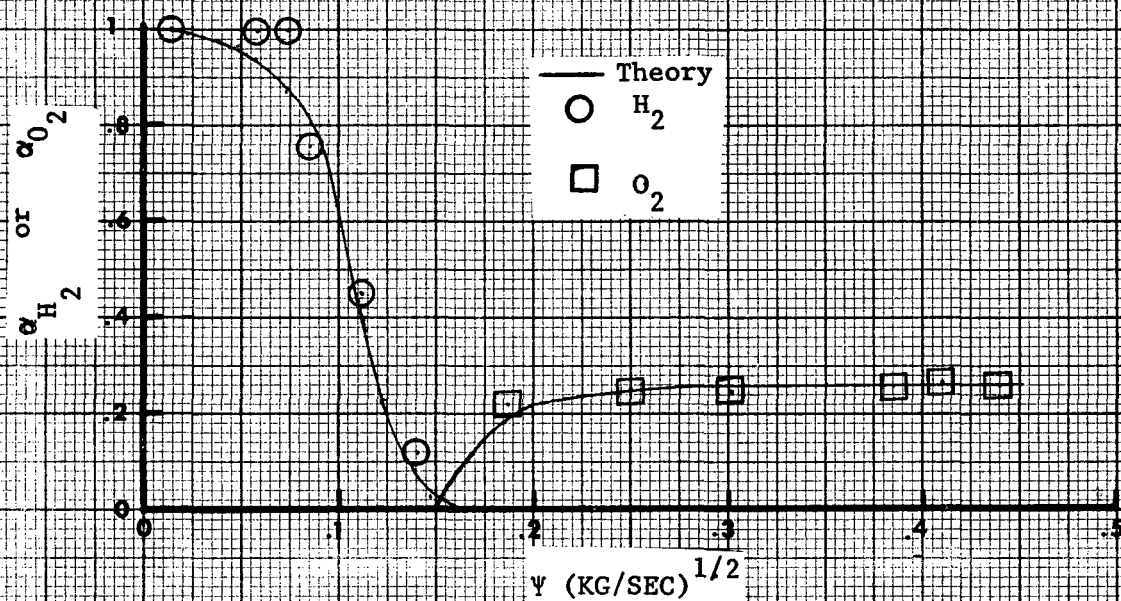
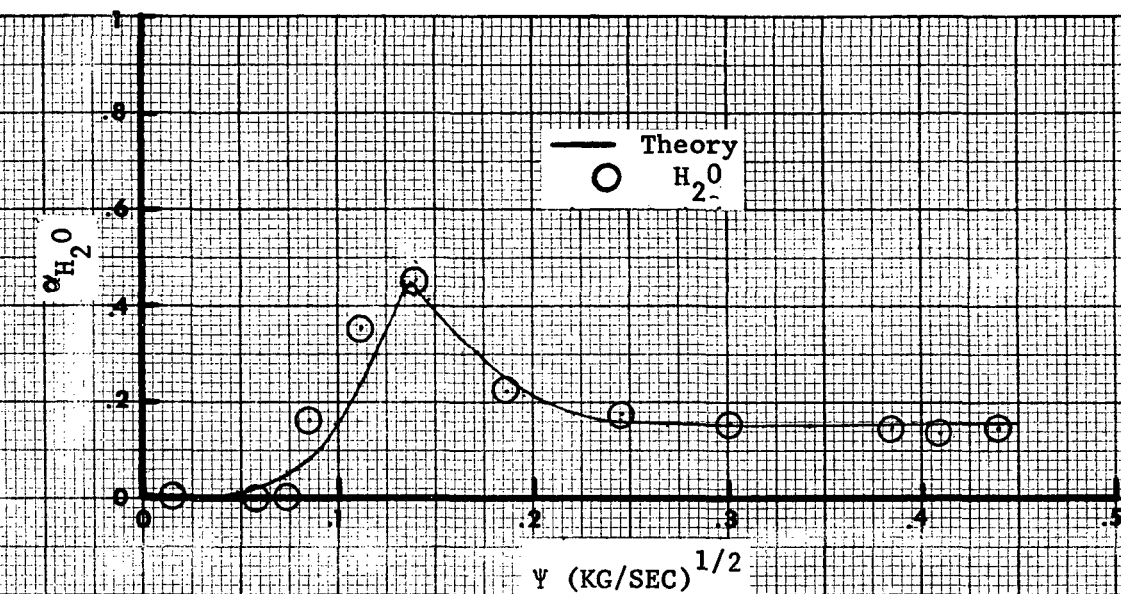
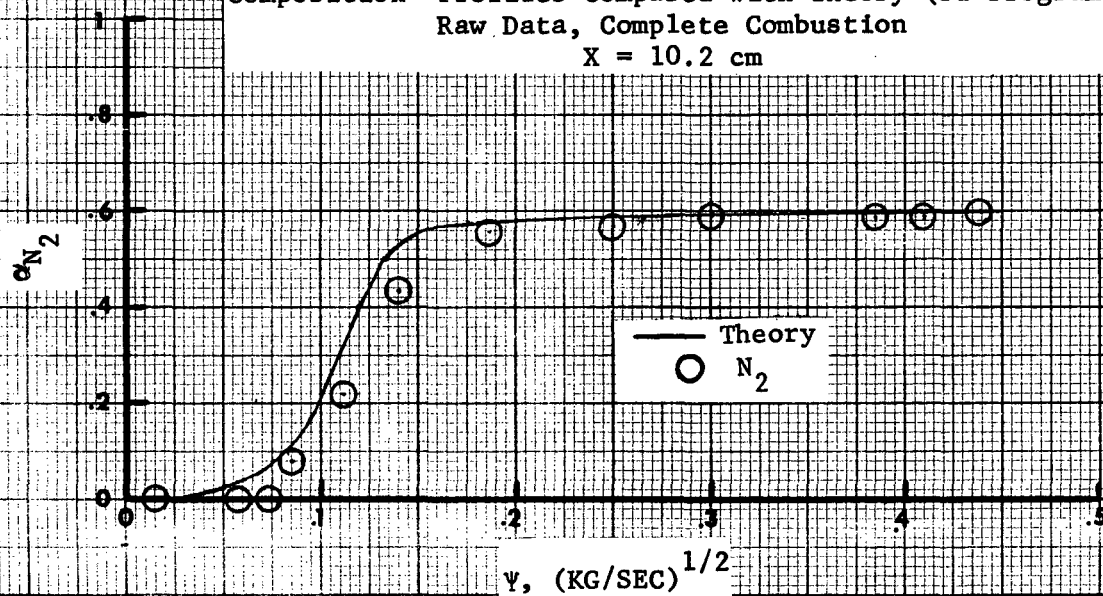


Figure 2.
Composition Profiles Compared with Theory (P1 Program)
Raw Data, Complete Combustion
 $X = 10.2$ cm



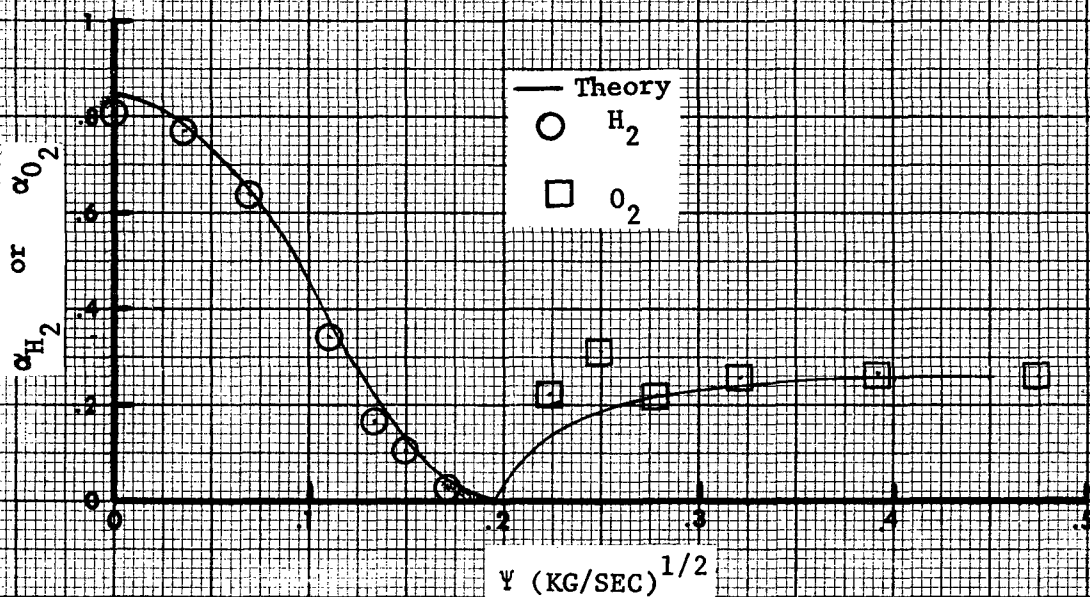
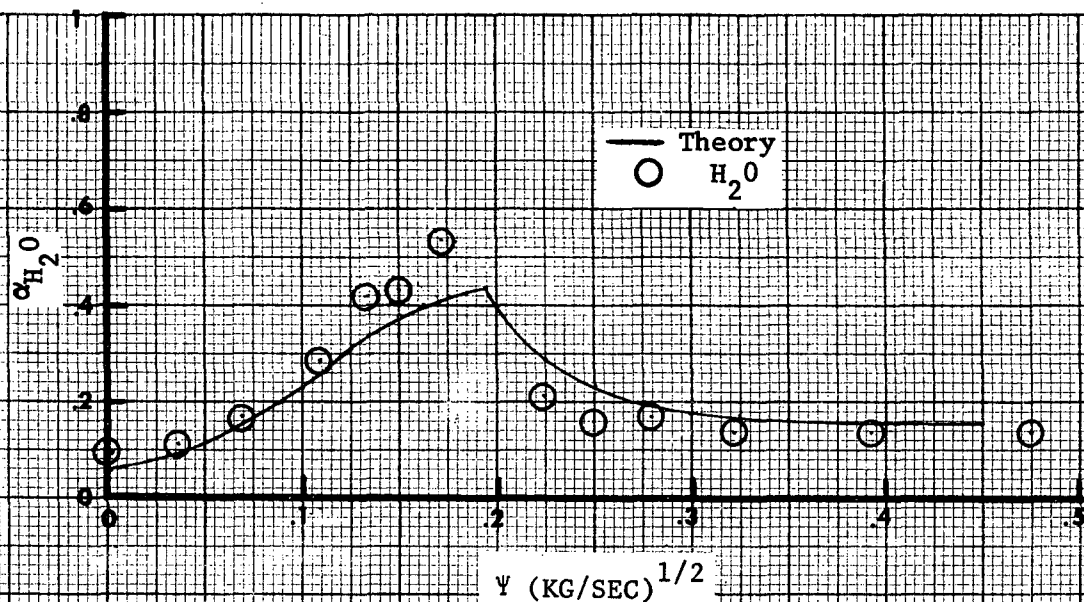
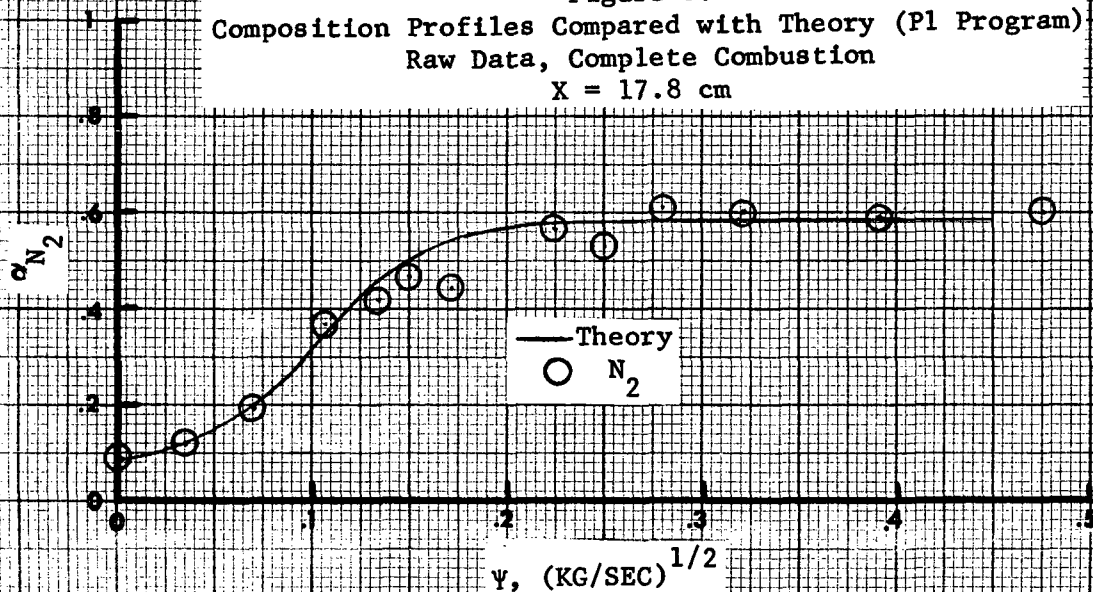


Figure 3.
Composition Profiles Compared with Theory (P1 Program)
Raw Data, Complete Combustion
 $X = 17.8$ cm



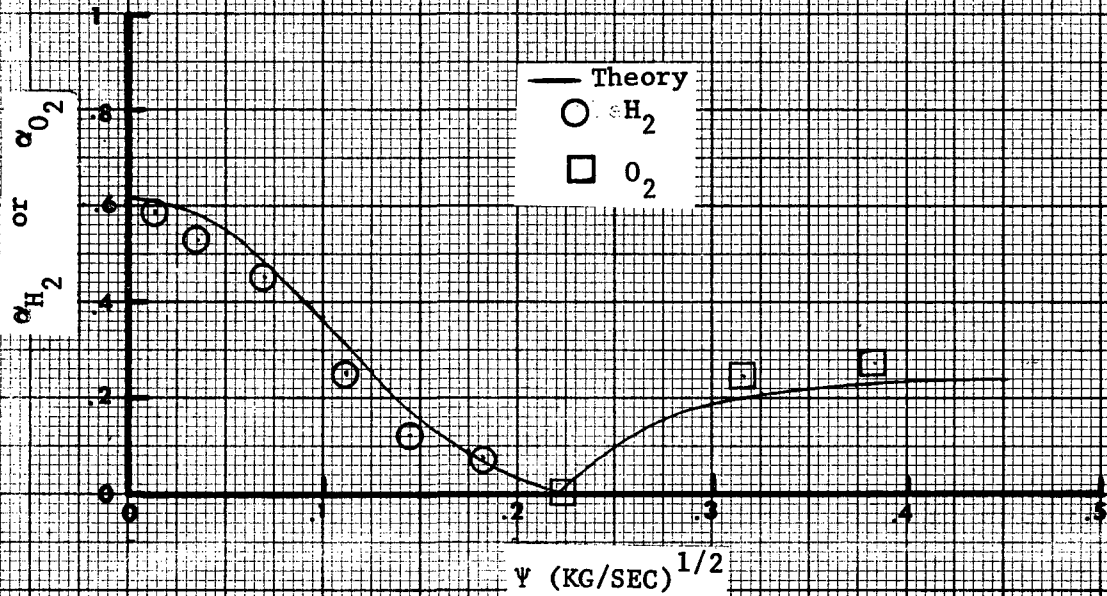
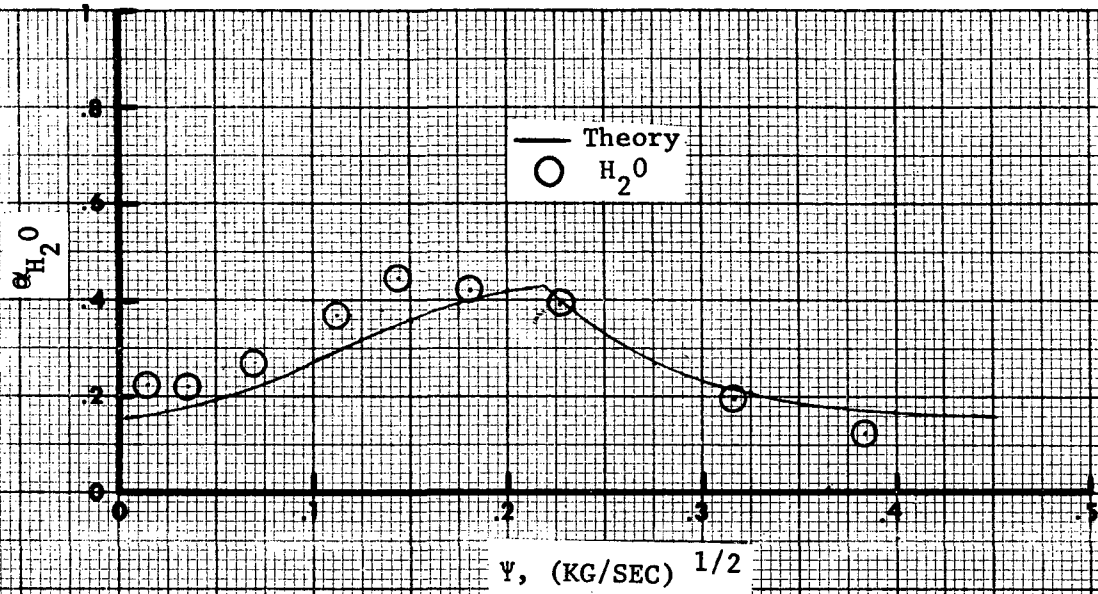
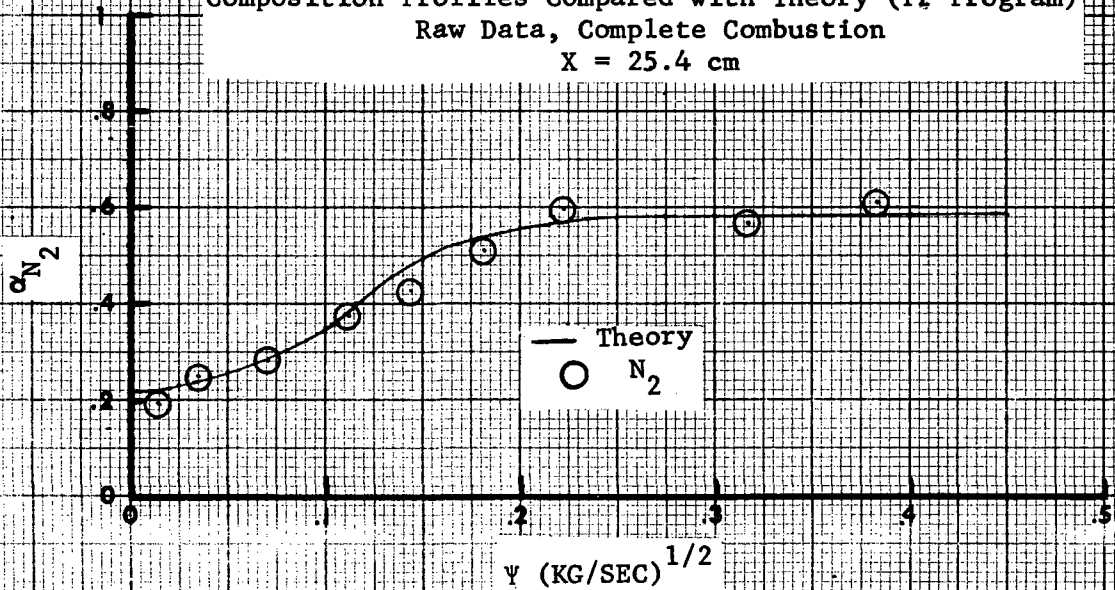


Figure 4.
Composition Profiles Compared with Theory (PI Program)
Raw Data, Complete Combustion
 $X = 25.4$ cm



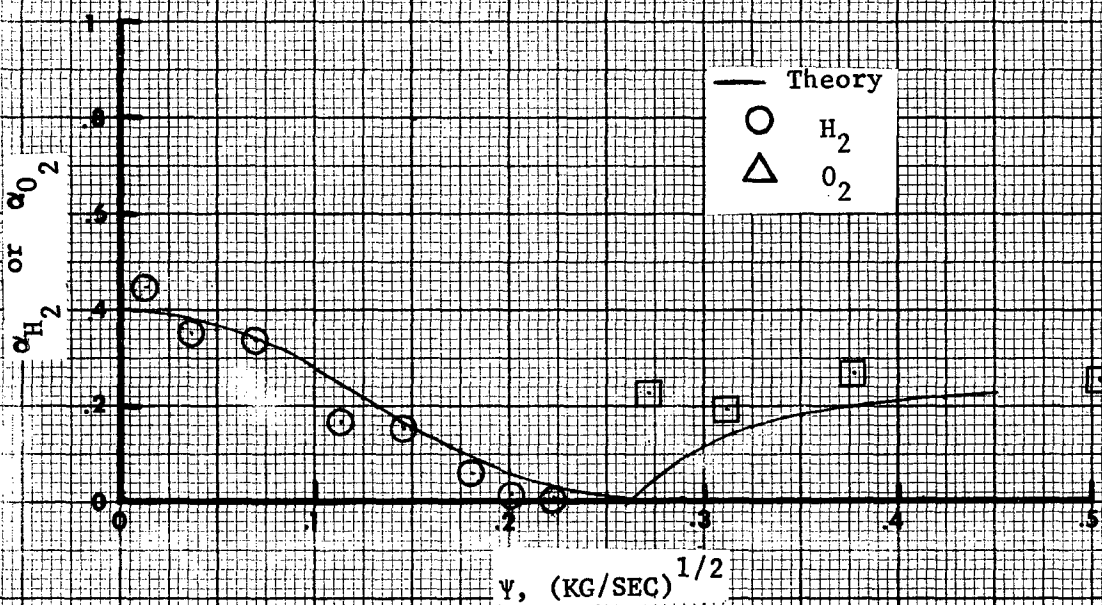
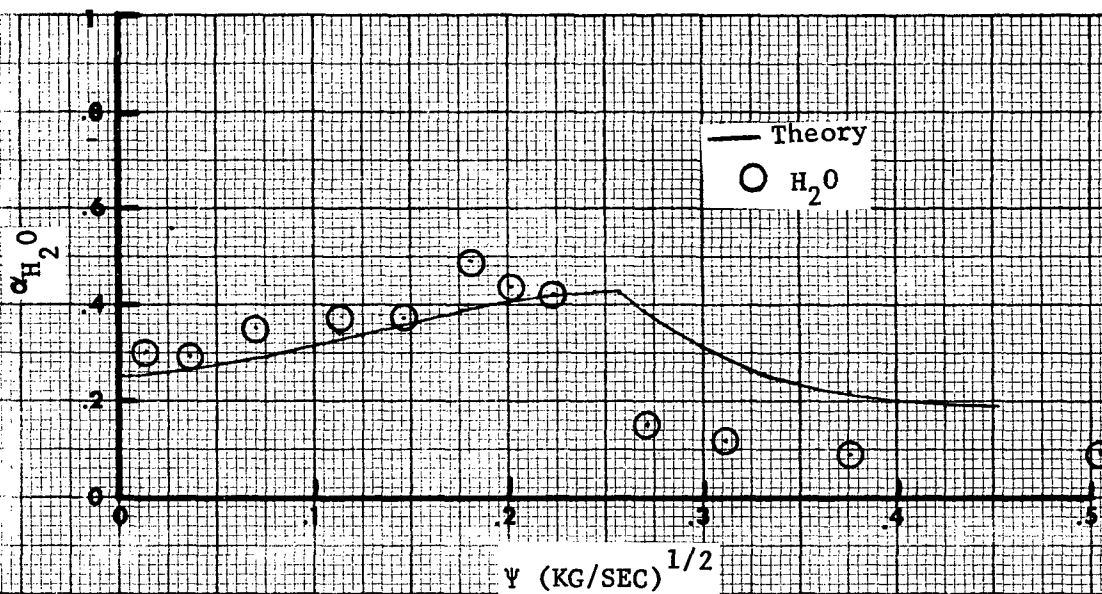
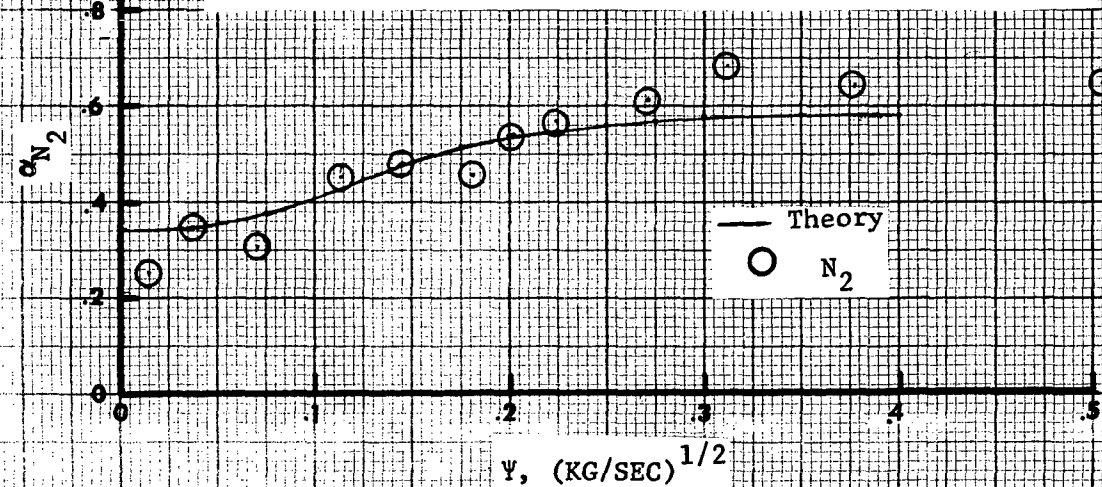
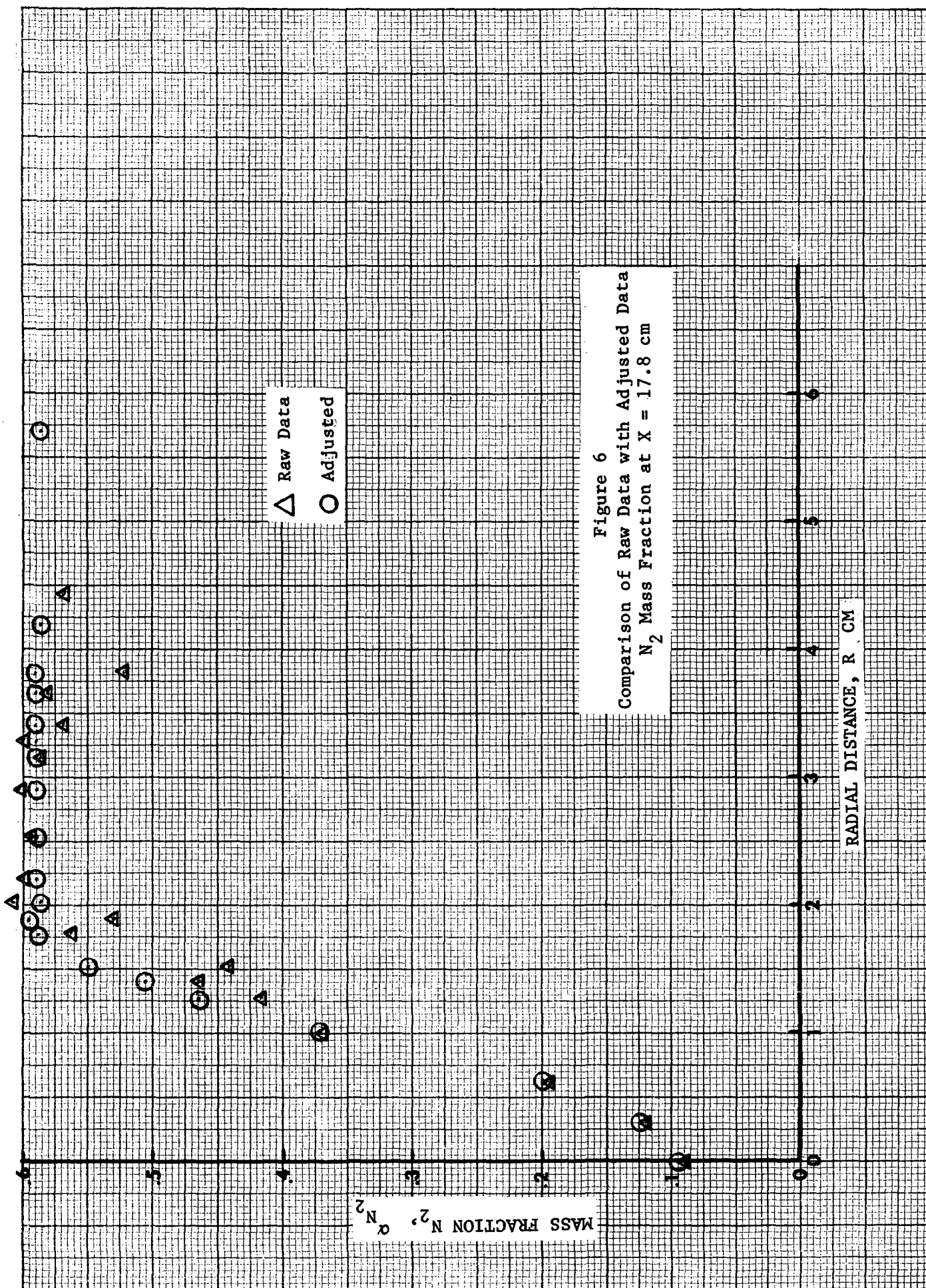
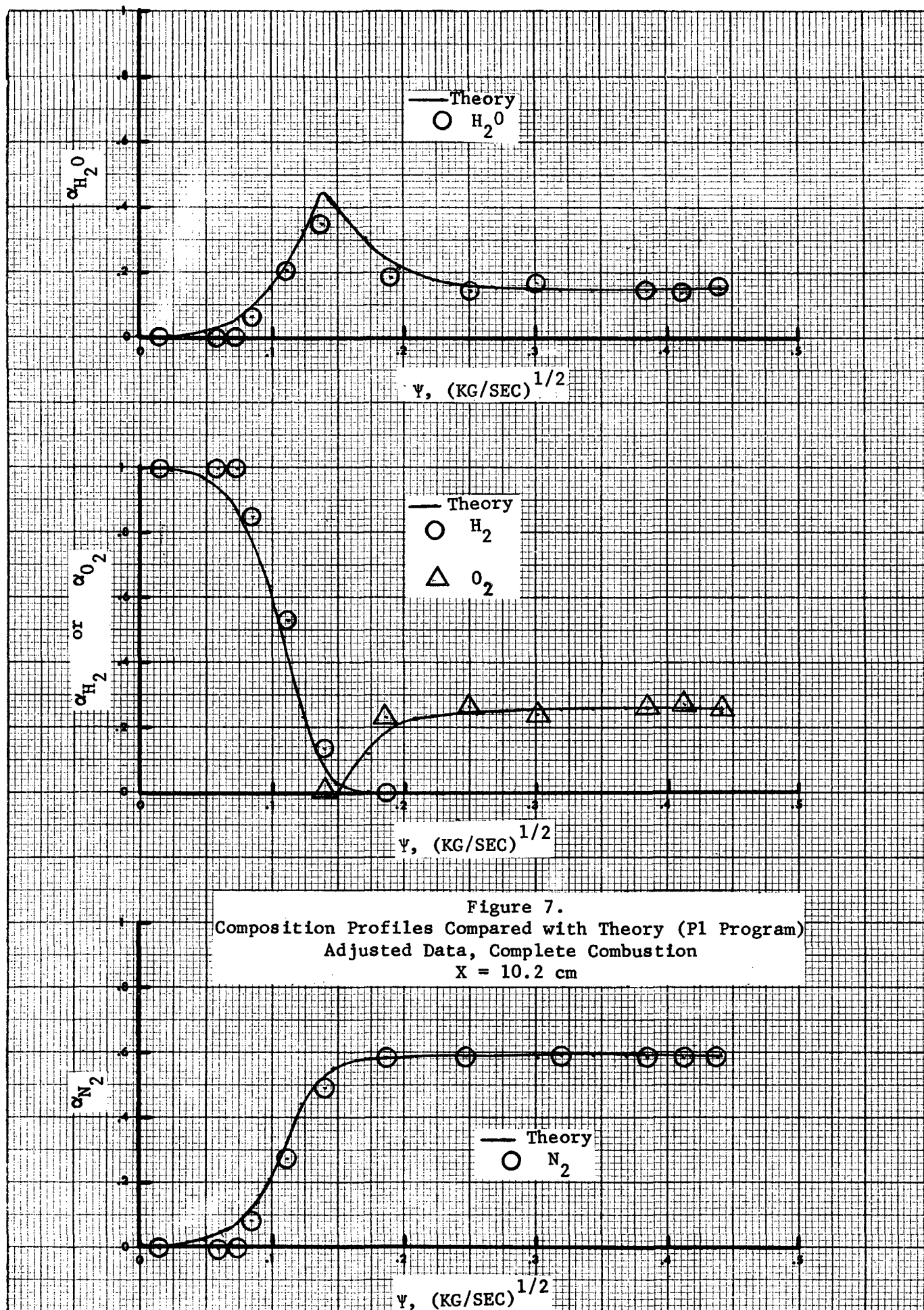


Figure 5

Composition Profiles Compared with Theory (P1 Program)
Raw Data, Complete Combustion
 $X = 35.6cm$







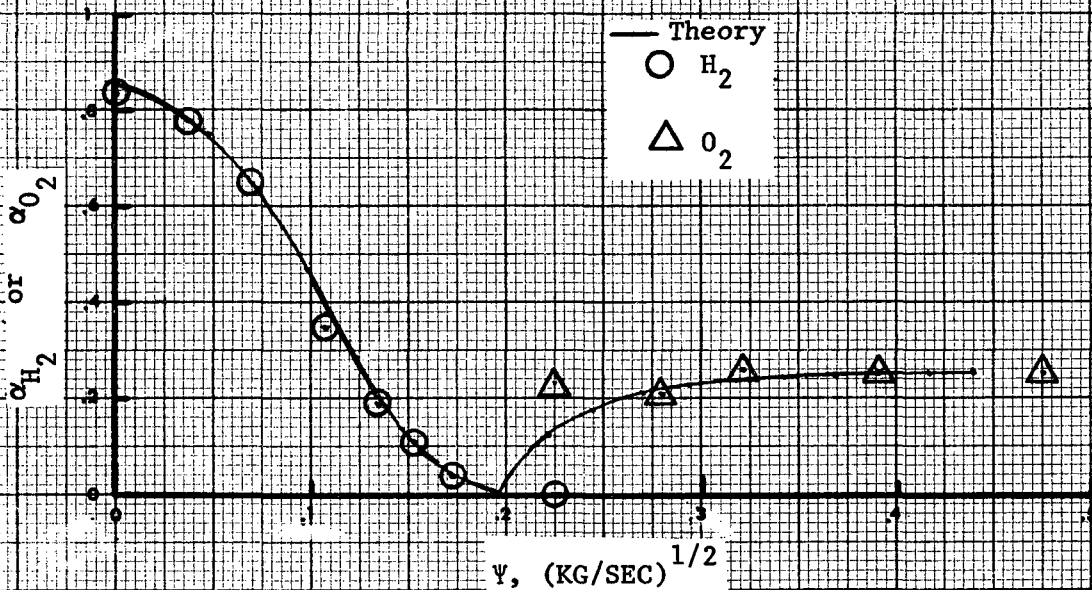
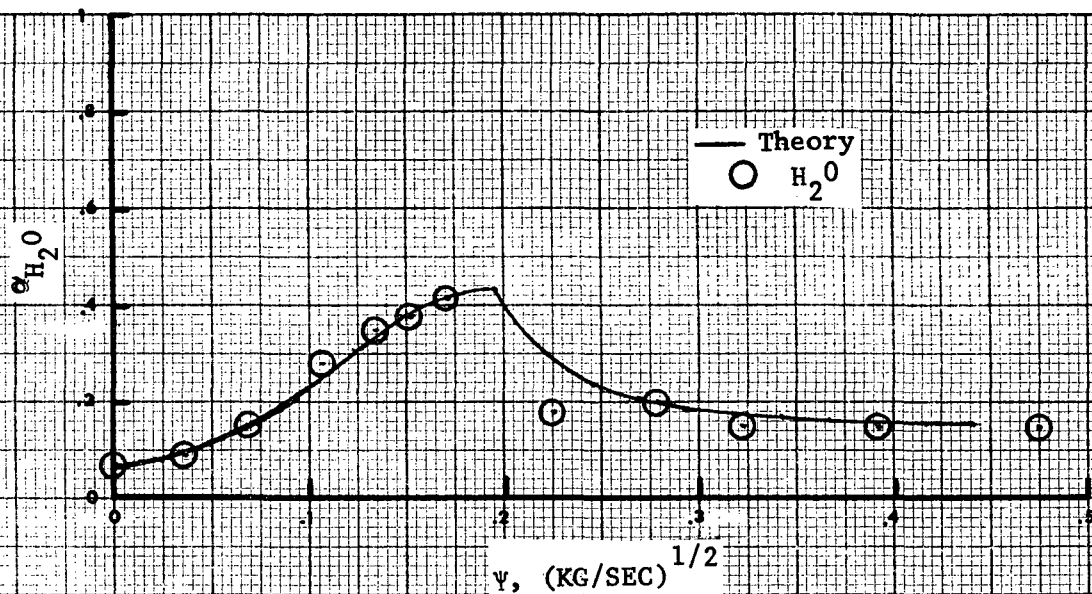
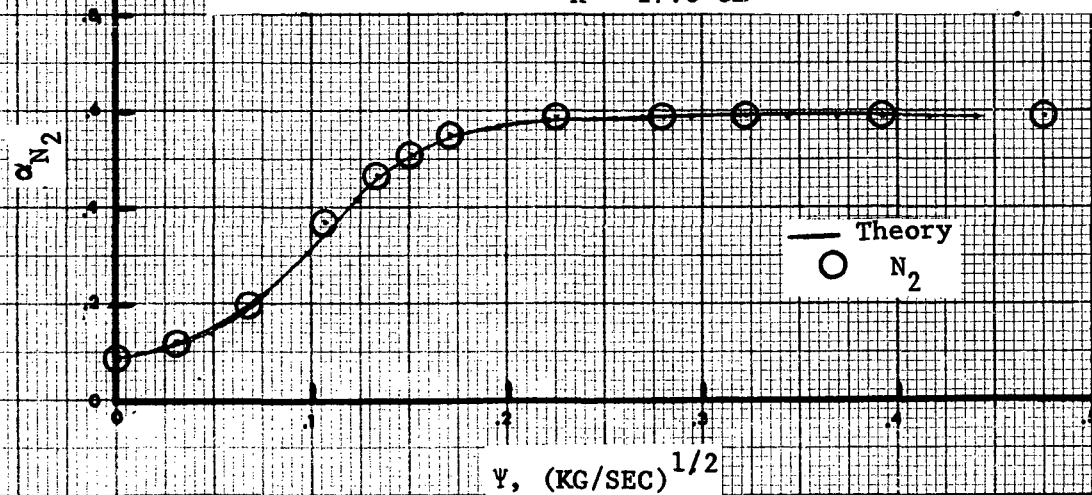


Figure 8.
Composition Profiles Compared with Theory (Pl Program)
Adjusted Data, Complete Combustion
 $X = 17.8$ cm



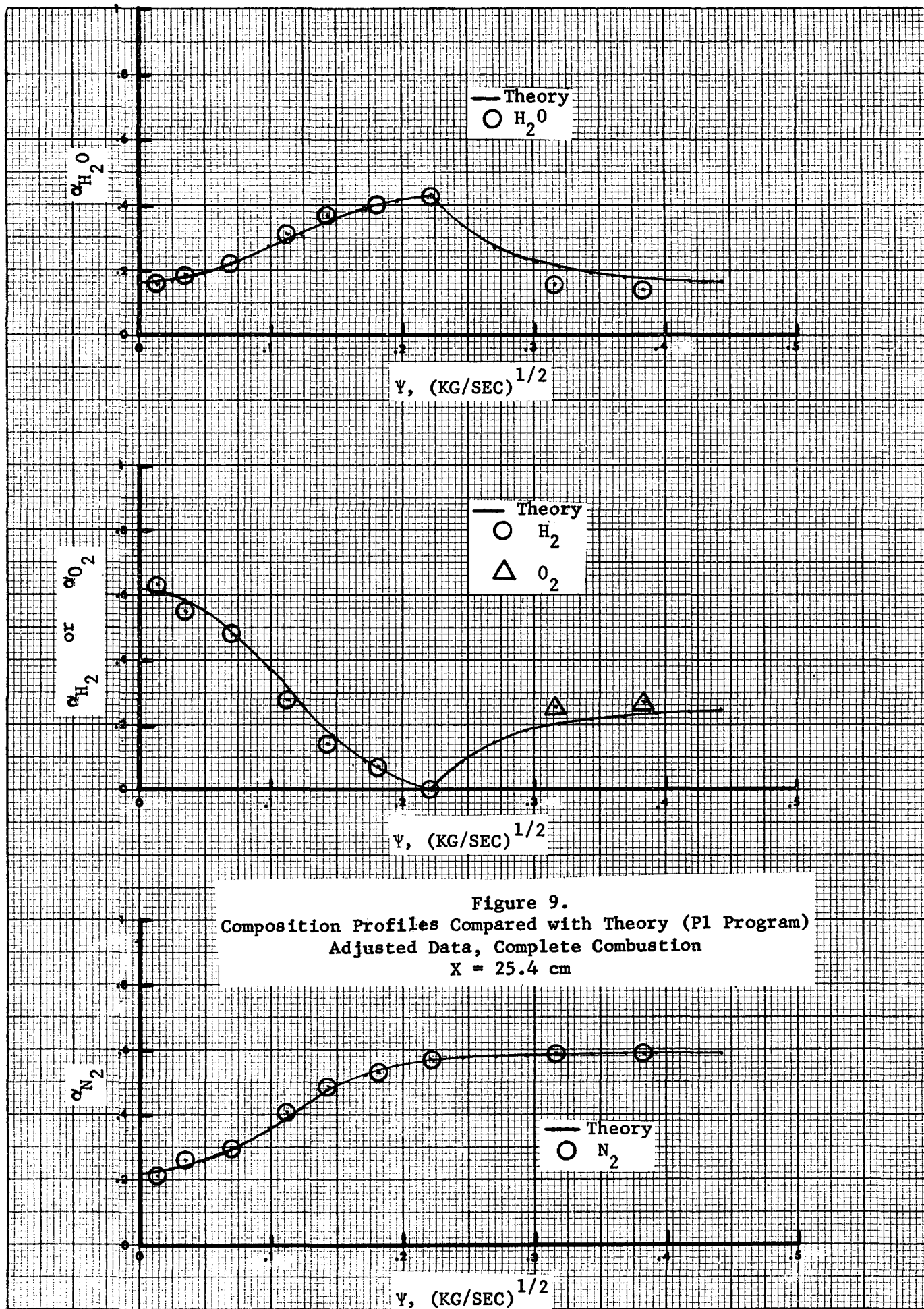


Figure 9.
Composition Profiles Compared with Theory (PI Program)
Adjusted Data, Complete Combustion
 $X = 25.4$ cm

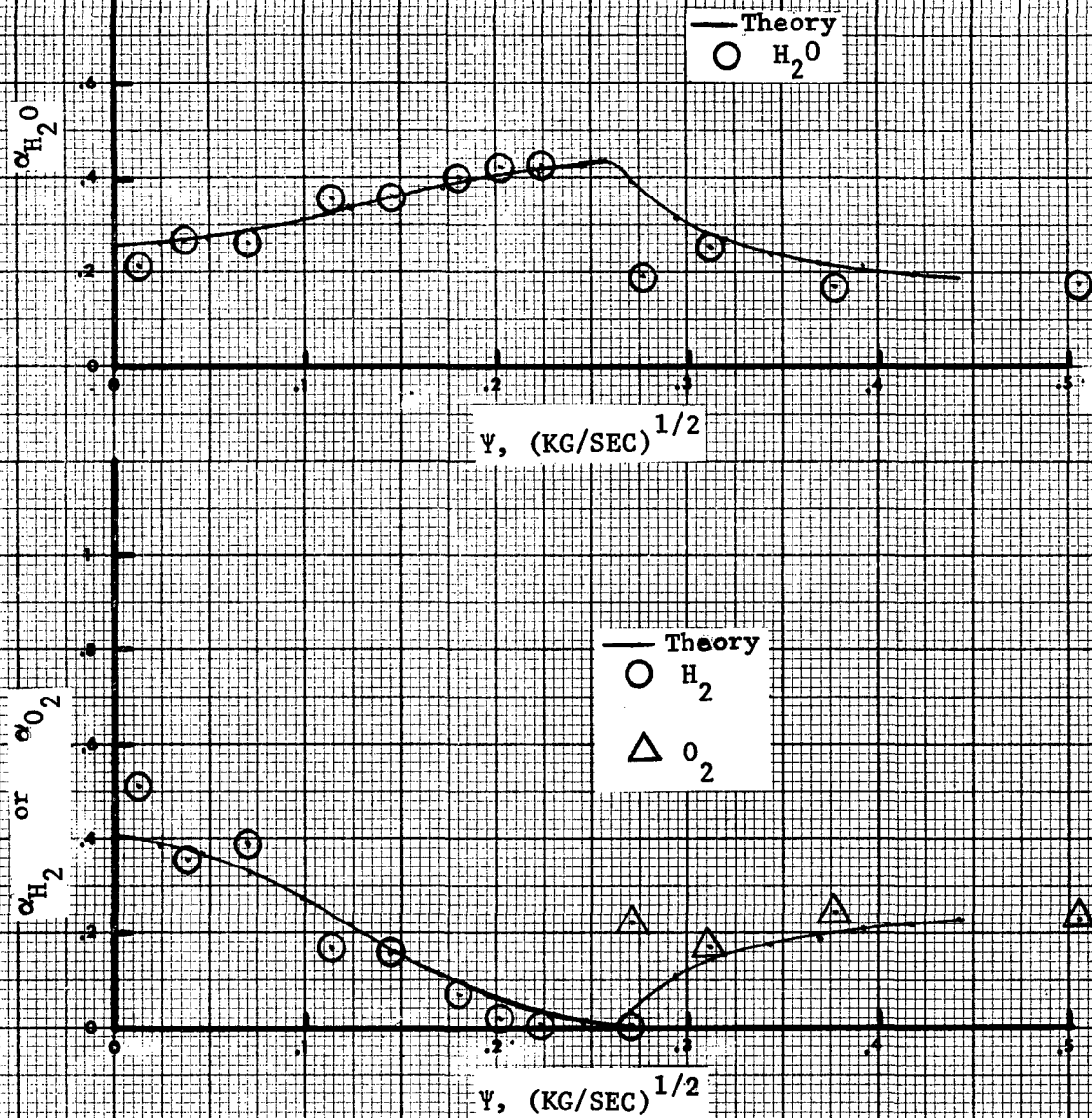


Figure 10.
Composition Profiles Compared with Theory (Pl Program)
Adjusted Data, Complete Combustion
 $X = 35.6 \text{ cm}$

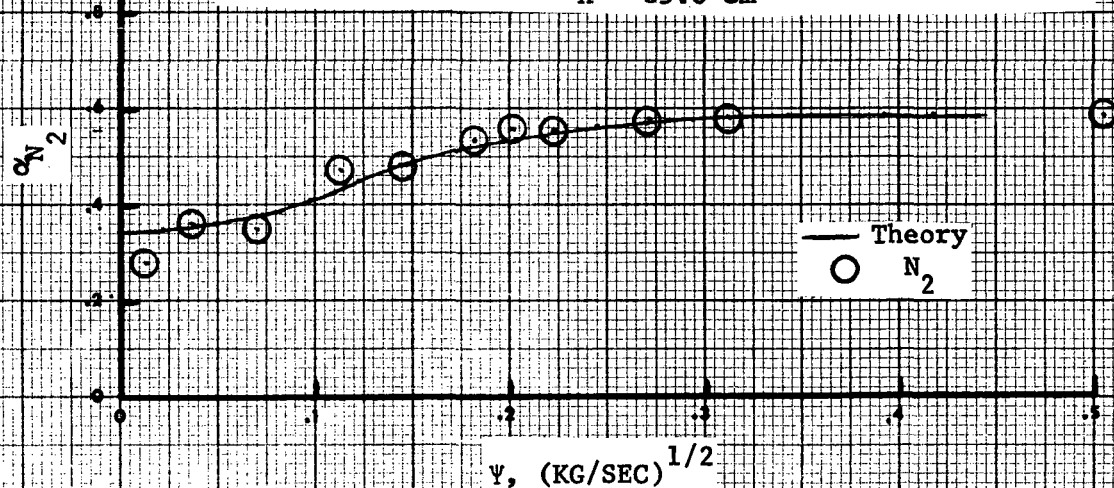


Figure 11
Composition Profiles Compared with Theory (H1 Program)

— Theory (Finite Rate Chemistry) $X = 8.02$ cm
○ Experiment (Adjusted Data) $X = 10.2$ cm

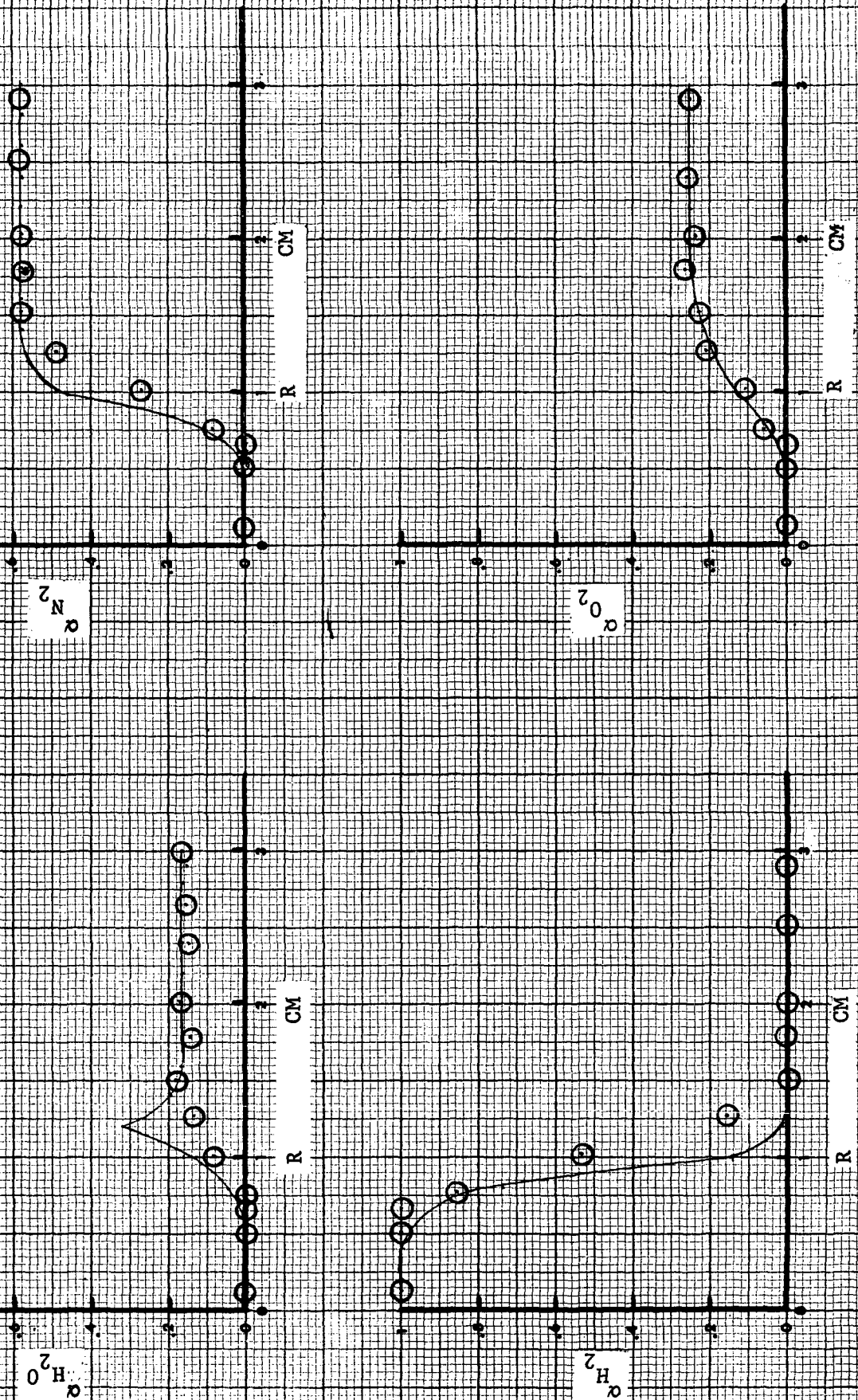


Figure 12
Radial Pressure Distribution (H1 Program)
Partial Combustion Chemistry; 1% Reaction per Step

$$P_0 = 0.91 \times 10^5 \text{ N/m}^2 (0.9 \text{ atm})$$

$X = 10.2 \text{ cm}$

$X = 17.8 \text{ cm}$

$X = 25.4 \text{ cm}$

RADIAL DISTANCE, R CM

P/P_0

P/P_0

P/P_0

Figure 13
Axial Pressure Distribution (H1 Program)
Partial Combustion Chemistry; 1% Reaction per Step

$$P_0 = 0.91 \times 10^5 \text{ N/m}^2 (0.9 \text{ atm})$$

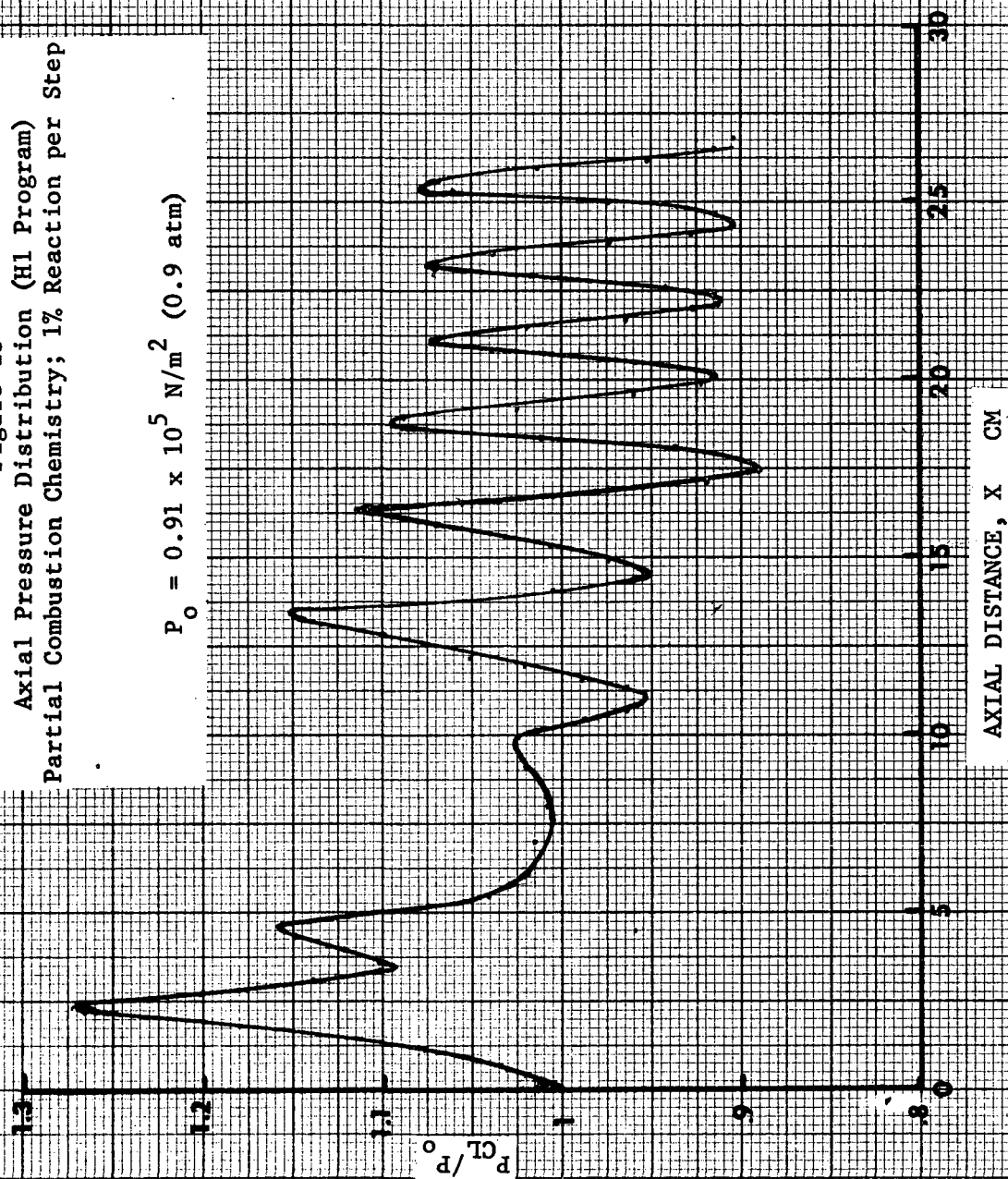


Figure 14
Radial Distribution of Water from Combustion
Partial Combustion Chemistry (1% Reaction per Step)

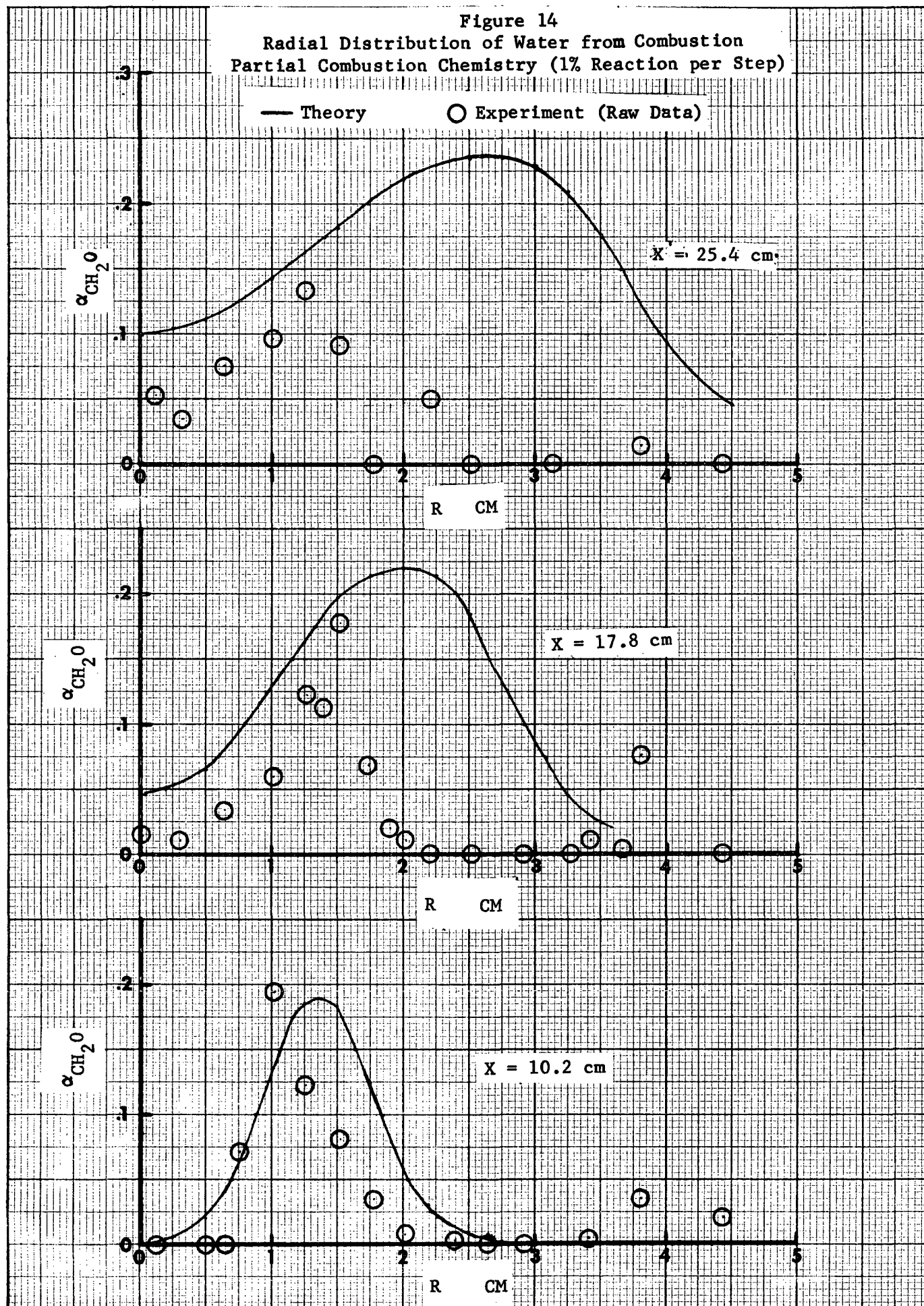


Figure 15
Radial Distribution of Water from Combustion
Theory H1 Program

— Total Combustion
----- Partial Combustion (1% Reaction per Step)

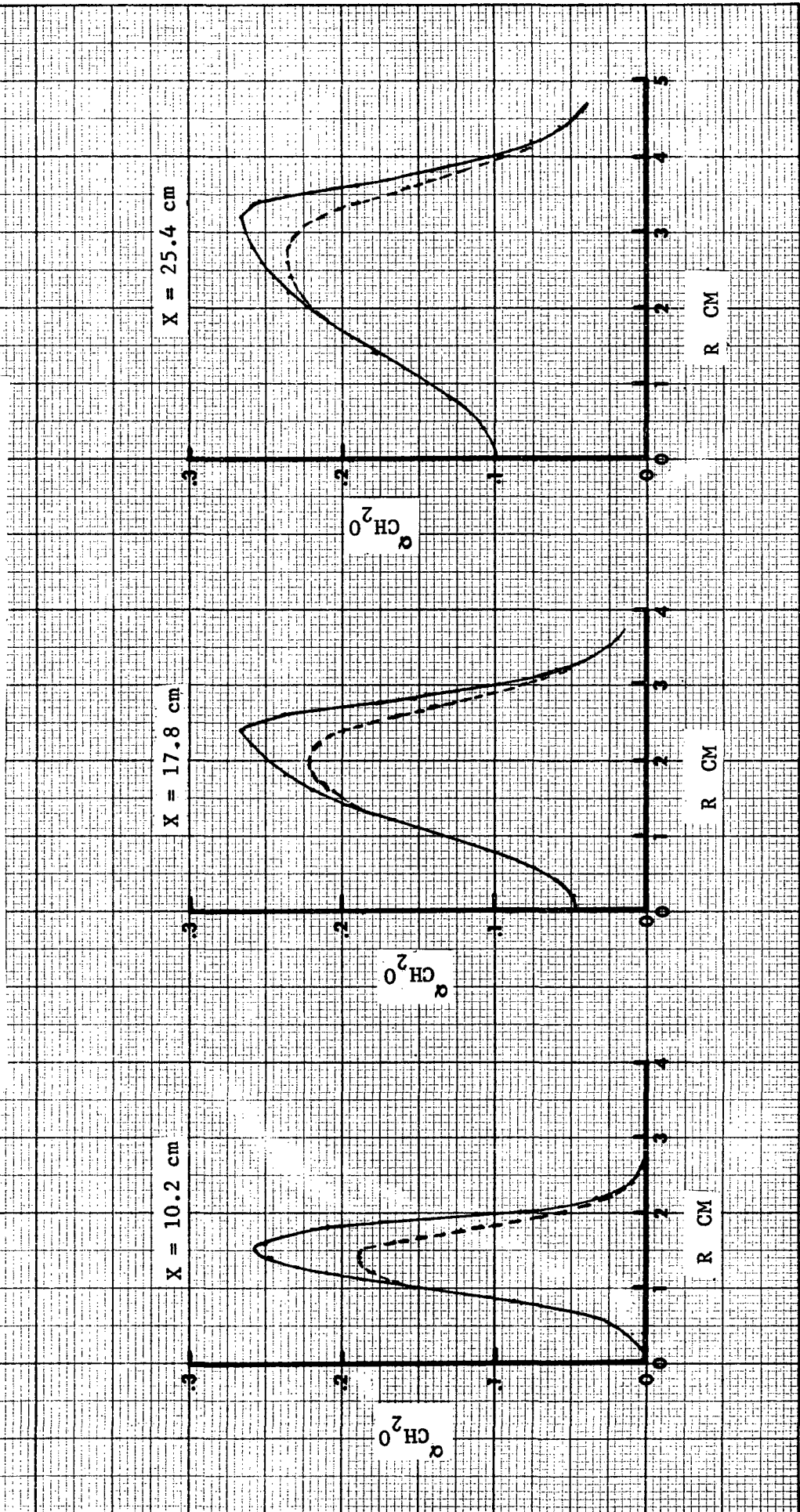
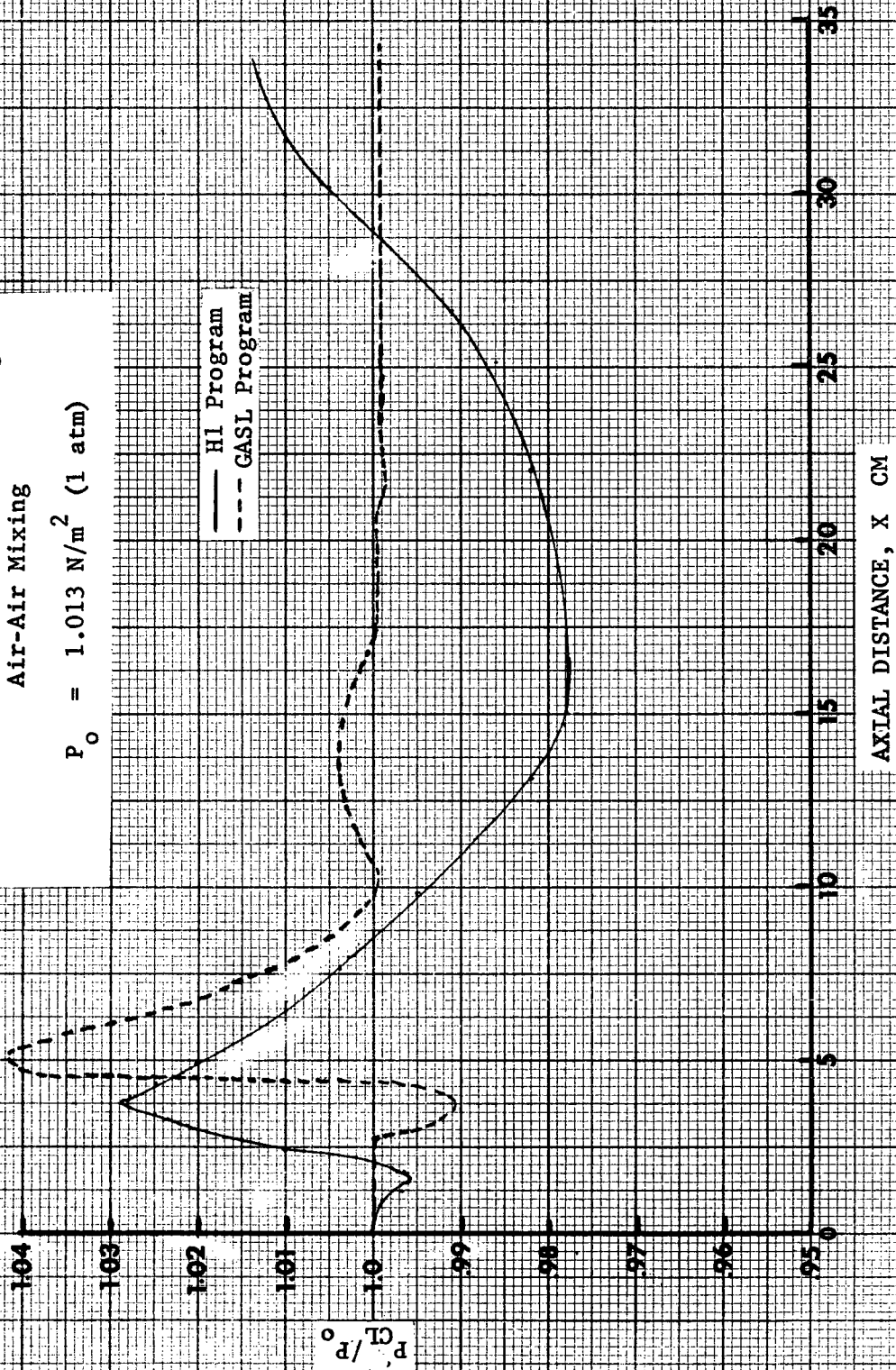


Figure 16
Axial Pressure Distribution (H1 Program)
Air-Air Mixing

$$P_o = 1.013 \text{ N/m}^2 (1 \text{ atm})$$

— H1 Program
--- GASL Program



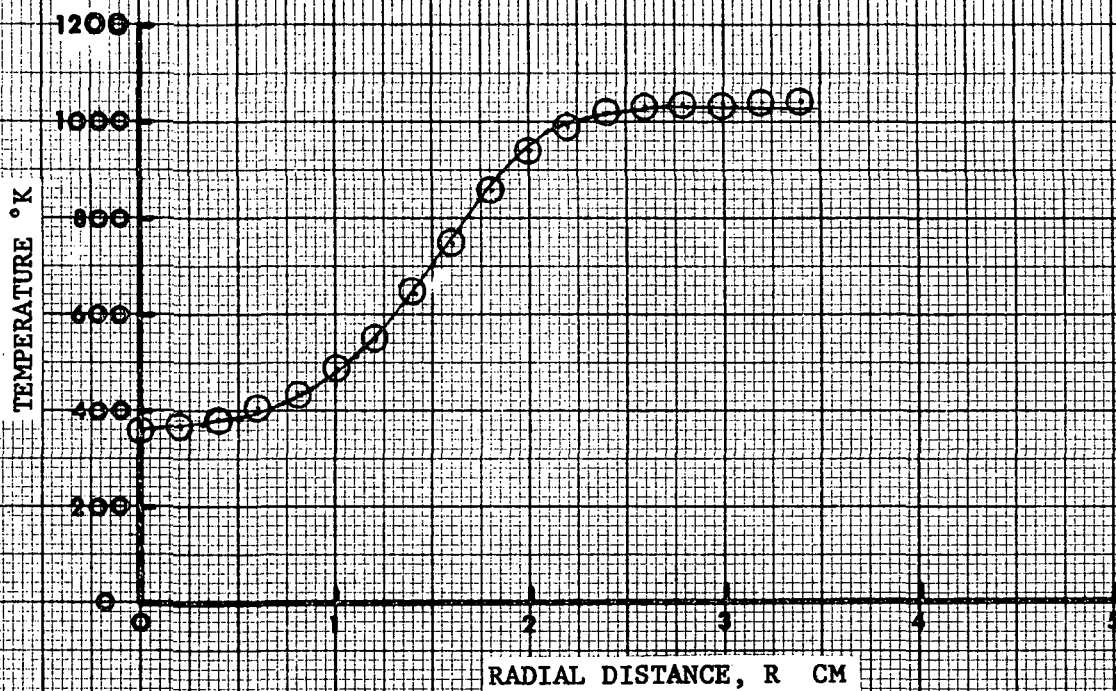
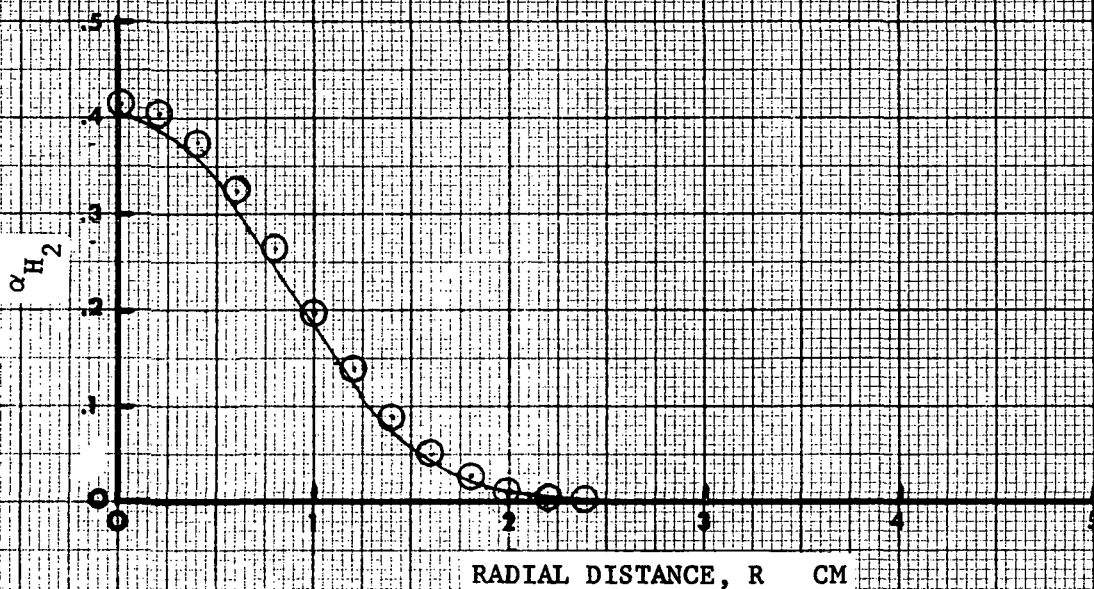
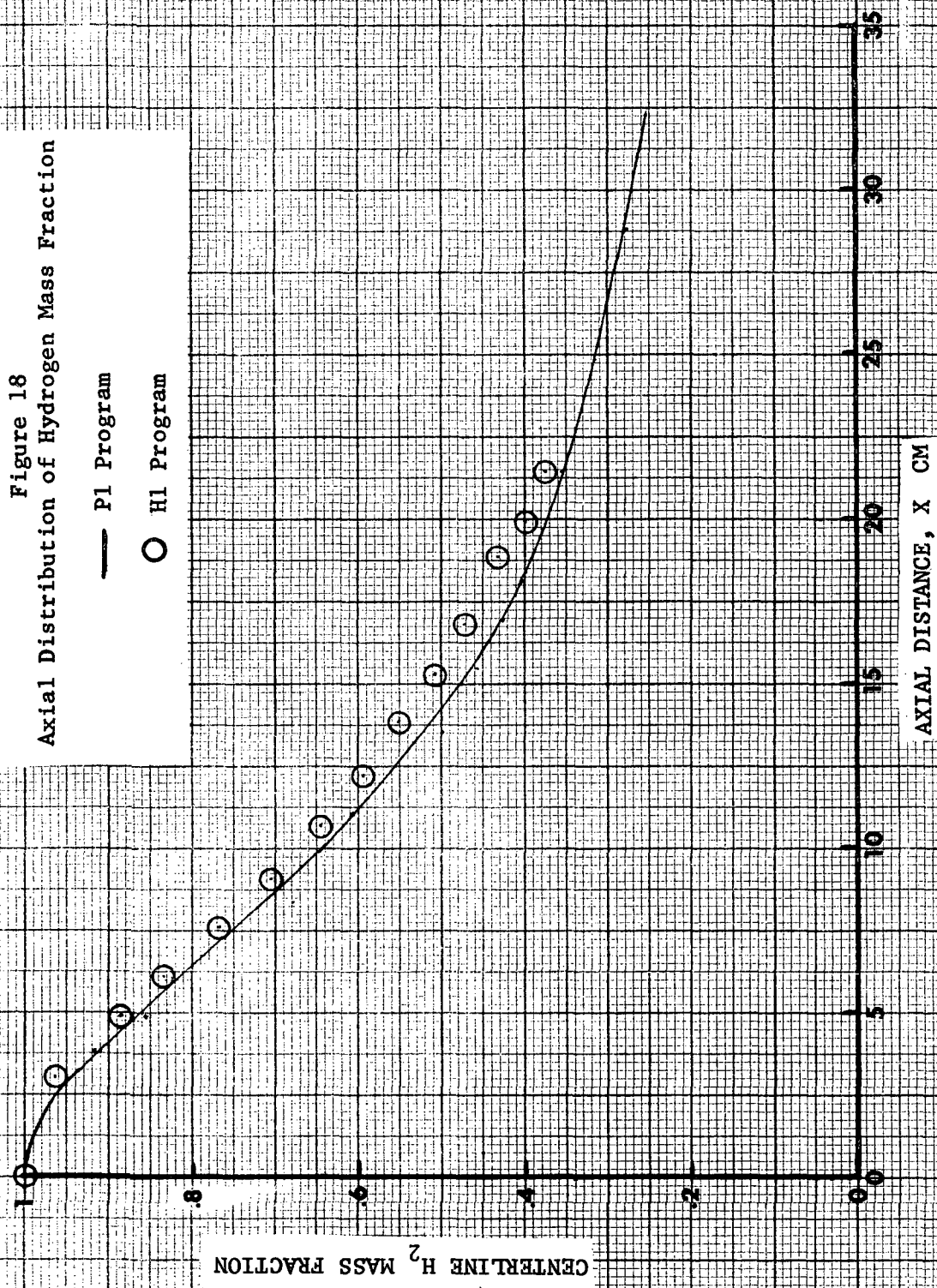


Figure 17
Radial Distribution
of
Temperature and Hydrogen Mass Fraction

— P1 Program
○ H1 Program
X = 18.32 cm





CENTERLINE H₂ MASS FRACTION

AXIAL DISTANCE, X CM