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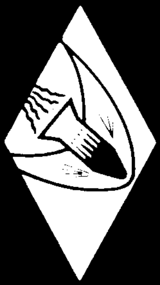

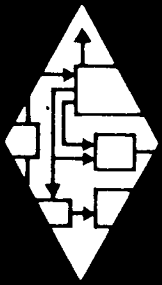

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INVESTIGATION OF COMBUSTION OF HYDROGEN IN A HYPERSONIC AIR-STREAM - FINAL REPORT

Technical Report No. 529

by S. Slutsky

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INVESTIGATION OF COMBUSTION OF HYDROGEN IN A HYPERSONIC AIR-STREAM

GASL TECHNICAL REPORT # 529

FINAL REPORT

S. Slutsky

Contract No. NAS8-2686

Prepared for

National Aeronautics and Space Administration
George C. Marshall Space Flight Center
Huntsville, Alabama

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ABSTRACT

A detailed investigation of the problem associated with the venting of combustible hydrogen from launch vehicles is summarized. Problems associated with the kinetics of the hydrogen air system ,including the two phase phenomena associated with cryogenic hydrogen, as well as the fluid mechanical mixing problems and the coupling of the two were considered. Experiments were performed in support of the many theoretical analysis.

It is concluded that the manner of hydrogen venting determines the combustion hazard. Results indicate combustion would occur if the venting were such that hydrogen could diffuse into the boundary layer on the vehicle surface.

In reaching these conclusions important technical capabilities in the fields of two phase flow, detailed compressible turbulent boundary layer studies, and practical techniques for computing flows with diffusion and finite rate chemistry were developed.

author

TABLE OF CONTENTS

ILLUSTRATIONS

INVESTIGATION OF COMBUSTION OF HYDROGEN IN A HYPERSONIC AIR-STREAM

I. INTRODUCTION

The advent of hydrogen fueled upper stage launch vehicles has created problems associated with the dumping of this combustible hydrogen during actual flight. Since the hydrogen will mix with the exterior air flow, the possibility of it combusting and releasing large amounts of heat energy in the vicinity of the vehicle has been investigated. To do so has required, first a description of the combustion process and second, a description of the flow field resulting from the mixing of the dumped hydrogen and the external air. The latter investigation yields information as to when and where in the flow field there will exist combustible mixtures of air and hydrogen.

Chemical kinetic studies were performed(Reference 1) to determine where in the launch trajectory conditions would be most favorable for combustion. Fluid mechanical mixing models were set up to investigate two dumping configurations; tangential slot injection, and injection by means of jets located parallel to, but removed from the vehicle surface. Initial studies considered simplified (linear) fluid mechanics with a simple (flame sheet) chemistry model (References 2,3,4). Both laminar and turbulent flows were investigated. More sophisticated flow models were then formulated requiring finite difference solution techniques and employing finite-rate kinetics models. (References 5, 6, 11, 14). Also investigated were the two-phase flow phenomena, i.e., condensation and evaporation, associated with the dumping of cryogenic hydrogen, (References 7, 8, 12, 13). These analytic formulations were supported by experimental investigations of both the slot and jet dumping configurations (References 9, 15).

Whereas conclusions drawn from the initial analytical studies indicated the probability of temperature and pressure fields too low to initiate combustion, experimental results indicated that combustion might indeed be possible. It was found that small disturbances, e.g., small surface protuberances in the vicinity of the hydrogen mixture could result in ignition of the hydrogen-air mixture. More sophisticated analytical investigation confirmed these observations.

Attention was next focused on the parallel jet dumping configuration. Experimental studies showed that the positioning of the jet, i.e., its distance from the vehicle surface, controlled the possibility of hydrogen diffusion into the vehicle boundary layer. Concurrent analytical efforts showed that hydrogen diffusing into the boundary layer could indeed combust in the neighborhood of the vehicle surface. It was further concluded that moving the jet far enough away from the surface would result in negligible hydrogen surface concentrations and hence to a negligible combustion hazard.

In the course of these studies, several important technical capabilities were developed. These are:

1. Analytical and numerical treatment of two phase flow systems including diffusion and finite rate chemistry.
2. Analytical and numerical treatment of the compressible turbulent boundary layer requiring no a priori assumptions of the compressible transport.
3. Practical computation techniques for the coupling of finite rate chemistry with diffusion.

Publications resulting from the above work are:

Edelman, R.E., Rosenbaum, H., "Generalized Viscous Multicomponent Multiphase Flows with Application to Laminar and Turbulent Jets of Hydrogen", AIAA Heterogeneous Combustion Conference, Palm Beach, Fla. December 11-13, 1963, also AIAA Journal Vol 2, No. 12, Dec. 1964.

Edelman, R.E., Rosenbaum, H., "Finite Rate Evaporation of a Cryogenic Propellant in a Binary Two-Phase Mixture with Application to the Hydrogen-Air System", AIAA 2nd Aerospace Sciences Meeting New York, N. Y., January 25-27, 1965.

Publications including significant contributions from the above work are:

Slutsky, S., Tamagno, J., Trentacoste, N., "An Experimental and Analytical Investigation of Ignition and Axisymmetric Turbulent Flame Propagation in Premixed Hydrogen-Air Flows with Application to Supersonic Combustion", AIAA 2nd Aerospace Sciences Meeting, New York, New York, January 25-27, 1965.

Ferri, A., Moretti, G., and Slutsky,S,, "Mixing Processes in Supersonic Combustion", SIAM National Meeting, Washington, D. C., May 11-14, 1964.

Ferri, A., "A Review of Problems in Application of Supersonic Combustion", Seventh Lanchester Memorial Lecture, May 12, 1964. Also Journal of the Roy. Aero. Soc. Vol 68 No. 645, September 1964 pp. 575-597.

II. TECHNICAL SUMMARY

The original statement of scope of work under the contract reads,"The Contractor will conduct analytical investigations of ignition characteristics of hydrogen in hypersonic boundary layers under combinations of static pressures and velocities typical of launch vehicle trajectories and of the heat transfer resulting from the chemical reaction. The flow configurations investigated are to be idealized to make them adaptable to analytic treatment".

In order to describe the generally complex physics of a reacting non-homogenous jet or boundary layer, the problem was considered by means of a succession of progressively more encompassing formulations of the physical model. In pursuing this approach there were carried out a number of studies which will be described in the following report.

The first study was summarized in GASL TR 330, entitled "Engineering Estimates of Flow Lengths Associated with the Combustion of Hydrogen-Air Mixtures During a Launch Trajectory", by P. A. Libby, H. S. Pergament, and P. Taub, Reference 1. In this study, estimates were made of the combustion characteristics of hydrogen ejected from a launch vehicle during a typical exit trajectory under the assumption of inviscid flow. The flow lengths associated with the induction (or ignition) period and the heat release (or reaction) period of the hydrogen-air reaction were computed. The first so-called "induction period" involves major alterations in composition (such as the formation of water and of intermediate species) with no significant heat release, i.e., no temperature rise. During the second reaction period, the concentrations of the intermediates decay and heat is released.

The times associated with both periods are readily estimated for a given pressure and initial temperature. It is therefore possible to apply such estimates to determine the flow lengths associated with the induction and heat release periods and thus to estimate under what flow conditions combustion in the vicinity of the launch vehicle can be expected. The estimates do not include delays due to vaporization of liquid fuel, intermixing of the hydrogen with the air or of phase changes in two-phase mixtures of gaseous and condensed oxygen, nitrogen, hydrogen.

During an exit trajectory there are two counteracting effects influencing the induction and combustion times. As the launch vehicle accelerates the static pressures near the vehicle decreases, tending to increase the induction times while the maximum static temperature behind strong shock waves increases, tending to decrease such times. Accordingly it might be expected that the estimated flow lengths would have a minimum. This was indeed found to be the case. Thus for injection schemes as shown Figure 1 and for a flight trajectory as given in Figure 2, it was concluded that dumping of hydrogen either through a slot or through a tube parallel to the free stream would give considerably longer combustion lengths than for normal injection. Critical altitudes were found to lie in the region between 125,000 and 175,000 ft. depending on the amount of injection. It should be noted that these first results were conservative (i.e., having shorter flames) since they did not take into account delay times due to evaporation, mixing, etc.

Next there were studied the effects of injection of hydrogen into a laminar boundary layer via a tangential wall slot. This work was reported in Technical Report 332 entitled "Slot Injection of Reactive Gases in Laminar Flow with Application to Hydrogen Dumping" by Paul A. Taub. (Reference 2). The work made use of a technique of linearization of the flow field and resulted in the formulation of a non-similar type of boundary layer associated with the initial value problem of heat flow theory. The idealizations of laminar and steady constant pressure flow were applied. The chemical behavior was taken to correspond to either frozen flow or to equilibrium flow. The equilibrium flow resulted in the possibility of using the flame sheet approximation. In addition, the assumption of Prandtl number and all Lewis numbers equal to unity was used. The product ρ times μ non-dimensionalized with respect to $(\rho\mu)_e$(exterior) was denoted by C and was taken to be a function of the streamwise coordinate only. Calculations were carried out for a typical launch trajectory at the point corresponding to the minimum delay time discussed in the above report. Thus, most of the calculations were performed at an altitude of 45 kilometers, an ambient temperature of 275° K and an ambient pressure of .00157 atmospheres. Vehicle velocity was 5800 feet per second. Heat transfer results for two cases with constant wall temperatures are shown in Figures 3 and 4. These curves are drawn for both equilibrium and frozen flow conditions. Additional calculations were made with several values of the ratio of jet velocity to external velocity and some with values of high exterior flow temperature corresponding to flow through an upstream shock. The results illustrate the advantages of injection of cold gases into the boundary layers of launch vehicles. In many cases, reactions may be assumed to occur but it was found that the heat transfer rise associated with combustion may be delayed for substantial distances downstream of the slot injector and the heat transfer rise may be relatively minor.

In connection with the above boundary layer program it was considered of interest to estimate the induced pressure forces associated with the boundary layers. It was found that the pressure coefficient was caused to increase at the forward portion of the boundary layer and to become negative further down along the boundary layer due to the curving back of the combustion region as the flame hits the structure. Details of the calculation and procedure are described in TR 365 entitled "Induced Pressure Forces Due to Hydrogen Dumping" by Harold Rosenbaum, (Reference 3). The procedure was relatively simple requiring only the computation of the displacement thickness and the subsequent determination of the pressure coefficient which was defined by linearized supersonic theory to be proportional to

$$\frac{d\delta}{ds} \bigg/ \sqrt{M_e^2 - 1}$$

In parallel with the above boundary layer problems the problem of flow in an axisymmetric jet was considered in TR 331 entitled "Axisymmetric Laminar and Turbulent Jets of Hydrogen With Simple Chemistry" by H. Rosenbaum. (Reference 4) The configuration considered here is that of a uniform axisymmetric jet of pure hydrogen issuing into a uniform parallel free stream. Both turbulent and laminar flow models with unity Lewis and Prandtl numbers were treated. The limiting chemical behaviors of frozen and equilibrium flow were assumed. The flame sheet approximation was applied in the case of the equilibrium model.

The calculations were performed along a point of a typical trajectory for a launch vehicle. The point chosen, was again, the 45 kilometer elevation. In the case of laminar flow the viscosity coefficient was computed in terms of the element values using the well known formula of Bromley. In the case of turbulent flow the eddy viscosity chosen was that suggested by Ferri, proportional to the difference $\rho_j u_j - \rho_e u_e$ times the characteristic scale equal to the half radius of the jet where subscripts j and e refer respectively to the jet centerline and free stream values. For the case of a jet temperature of 265°K the three values of the velocity ratio .33, .5, .8 were chosen; a jet temperature of 60°K and the velocity ratio of a half was also considered. Figures 5 to 8 show a flame sheet attained by the model for both turbulent and laminar equilibrium flow for the flight and gas conditions cited above.

It is of interest to note that for a given set of flight conditions there appears to be a dimensionless flame length that is virtually independent of the jet velocity to free stream velocity ratio U_j/U_e. For laminar flow the length of the flame sheet seems to be proportional to the square of the jet radius a^2 and to the first power of $\rho_j U_j/\rho_e/U_e$. For a turbulent flow, the flame length varies as the first power of the jet radius and the square root of the mass flux ratio

$$\frac{\rho_j u_j}{\rho_e u_e}$$

A comparison of the flame lengths encountered in laminar and turbulent flow for conditions considered here indicate a ratio of the order of 100 to 1, (laminar to turbulent).

The foregoing work was concerned primarily with the development of estimates of the effect of hydrogen dumping on the heat transfer through the boundary layer of the launch vehicle. Accordingly limits of these heat transfer effects were determined using such approximations as frozen flow for relatively slow reaction conditions and equilibrium flows for relatively fast reaction conditions. The effect of turbulence was gauged using simple transport models.

In the next phase of the work our goal was extended to develop an understanding of more realistic aspects of hydrogen dumping from launch vehicles. Thus, the program was concerned with conditions for ignition and combustion in the boundary layer of a non-homogeneous mixture of hydrogen and air as well as in the free field behind regions of shocks such as would be generated at conical transition sections. An estimate of the effect of solid or liquid phase components in the ejected hydrogen on the heat transfer and on the ignition characteristics of the mixture was considered in this phase.

TR 385 entitled "The Laminar Boundary Layer in Hydrogen Air Mixtures with Finite Rate Chemistry" by Libby, Rosenbaum and Slutsky (Reference 5) constituted an initial step in the development of a computer program which was conceived of having the capability of treating arbitrary laminar boundary layer flows with chemical reactions and accurately described transport properties. The flow field was related to the slot injection of hydrogen with a velocity equal to that in the external stream with simple transport properties and with constant pressure. The model was constructed starting with a Levy-Lees transformation of the fluid dynamic equations and with the assumption of the Blasius velocity profile. The $\rho\mu$ product was taken independent of the normal coordinate together with unit Prandtl and Lewis numbers. The finite rate chemical reaction mechanism and equations were the same as those used in the earlier work by Libby, Pergament and Taub, (Reference 1). Nitrogen was assumed to be an inert diluent and the reaction steps considered for the hydrogen-oxygen system were eight forward and eight reverse reactions. The diffusion coefficient associated with the diffusion of each of the species in the mixture was assumed to correspond to a Lewis number equal to unity. It is to be noted, that the assumptions of constant $\rho\mu$ of a single diffusion coefficient and of a similar velocity field were not essential to the numerical analysis and were chosen as a first approximation to a system of greater generality.

It was found that the finite difference program, as developed above, worked satisfactorily only when the chemical reactions were slow, that is when long ignition distances prevailed. With that restriction computation time for boundary layer distances over which the hydrogen mass fractions became negligible throughout the boundary layer was approximately 30 to 40 minutes. Thus, a program of utility in connection with heterogeneous but non-reactive flow was available. However, when the reactions were fast enough to lead to significant chemical production it was found that a streamwise step size had to be taken so small that computation was impractical. The difficulty was studied and was found to be associated with a "stiffness" of the equations controlling the free radical generation, i.e., of H, OH and O. The solution to this problem was found in subsequent work which is described later in this summary report.

Calculations with this program were carried out for points on the trajectory corresponding to an altitude of 45 KM and a Mach number of approximately 5, which gave a minimum ignition delay time and hence represents conditions most favorable for the combustion and heat release of the slot injected hydrogen. In addition, a case in which the external conditions of the boundary layer flow corresponded to that due to an oblique shock wave upstream of the slot was considered.

Numerical cases considered were denoted as cases 1, 2 and 3. Case 1 corresponded to a simple external flow over a flat plate whereas, cases 2 and 3 corresponded to conditions behind a 45° and 60° oblique shock. In all cases the wall or skin temperature was assumed to be 500°K. The temperature of the slot injected hydrogen was taken to be 75°K for case one and 100°K for cases 2 and 3. Under the idealization and assumptions underlying this study the numerical finite difference, finite rate chemistry calculations indicate no combustion in the boundary layers in the case of 1 and 2, within lengths of practical interest. In case 3, on the other hand, the program indicated the onset of reaction in a length in the order of 10 slot heights. The initial mass fraction concentrations and stagnation enthalpy profiles were obtained from the starting solution which was developed in Report 385. This starting solution technique was required in order to describe the development of the mixing region from the original slot lip, across which there exists a discontinuity in the temperature and mass fractions. There also exists an indeterminancy at the original lip region which was removed by a method due to Lu Ting, i.e., by equilibrating the second order pressures which result from the growth of the viscous mixing region emanating from the lip and its interaction with the boundary layer at the base of the flow.

It is interesting to note that the static temperature "pop" associated with the temperature distribution in normal air boundary layers does not exist in this flow. This is attributed to the cooling effect of the cold, high heat capacity hydrogen which, in a laminar mixing model, exists along the wall for distances large in comparison to the length of bodies of interest. Indeed, one first begins to notice this temperature "pop" on the order of thousands of feet (laminar flow) downstream of the injection point. Hence, under the idealization of the flow presented here, at no place in the fields of the cases 1 and 2 boundary layers do static temperatures of the order of the hydrogen air-ignition temperature appear, therefore no combustion is observed for those cases. Although unable to proceed into the combustion region, in Case 3 the program did predict the onset of reaction at a distance of the order of 10 slot heights. At that point the generation of reactive species was noted but the time required for the computer program to proceed became so large that the computations had to be halted. Conceptual modifications, as noted below, had to be applied before this program would operate satisfactorily in the region of rapid chemical combustion.

On the basis of observations made by A. Ferri in connection with supersonic engine hydrogen combustion studies, it is believed that local pressure perturbations due to combustion could be amplified by external flow field curvature induced in the case of the jet by local jet spreading and in the boundary layer by local boundary layer thickening. The pressure perturbations in turn speed up the chemical reactions in the perturbed region. Accordingly, a preliminary investigation of a first order interaction theory of pressure variation due to growth of the boundary layer displacement thickness coupled with combustion heat release was initiated. The mathematical statement of the problem was formulated using integral methods and was presented in GASL TR 377 entitled" A Preliminary Analysis of a Reacting Boundary Layer with Coupled Pressure Interaction" by R. Edelman and P. A. Libby (Ref. 6). In this analysis the external pressure was assumed to depend linearly on the slope of the displacement thickness in accordance with the linearized supersonic approximation. Simple transport properties were assumed with all Lewis and Prandtl numbers taken equal to unity. A moment method of solution was applied which is an extension of the Karman-Polhausen technique involving the use of the normal coordinate as a weighting function. There resulted a large system of first order non-linear ordinary differential equations. Although the equations for the hydrogen-air system were worked out in considerable detail the numerical work on the program was not followed through because of the considerable complexity of the equations and of the program that would be required to implement them. A more feasible formulation of the problem was subsequently proposed.

One of the obvious questions which must be asked in connection with the dumping of extremely cold hydrogen gas is whether or not there exists a possibility of condensation of the hydrogen or of the nitrogen and oxygen from the exterior flow and the effect of the condensation and subsequent evaporation on the flow field. We would like to be able to interpret the appearance of the observed vapor plumes in terms of the analytical predictions concerning evaporation and condensation. We would like also to know the implications of the condensed phases on the possibility of combustion and on the appearance and other gross phenomena associated with combustion in the presence of such condensed phases. In TR 349 entitled "Generalized Viscous Multicomponent Multiphase Flow with Application to Laminar and Turbulent Jets of Hydrogen" by Edelman, Rosenbaum and Slutsky, (Reference 7), a model was established for the continuum flow of a multicomponent system of gases and of their condensed phases.

In the numerical example treated, the boundary conditions were such that the flow was chemically frozen while phase transition was assumed to take place in equilibrium. This postponed the complication of rate chemistry and permitted this preliminary analysis to focus on multiphase effects. (The effect of rate chemistry is taken up in Report TR 508 discussed below.)

Numerical results for diffusion of an axisymmetric jet were presented. Figures 9, 10, and 11, show the jet geometry and the radial distributions of the pertinent variables at a representative streamwise station for an altitude of 40KM. Figure 9 is a schematic representation of the axisymetric jet showing a cone composed essentially of undisturbed two phase hydrogen. In crossing this cone boundary the hydrogen flashes to vapor in accordance with the equilibrium assumption. The remaining figures show the radial and axial distributions of mixture mass fractions of condensed phase and gas phase components. In addition temperature and velocity distributions are presented.

The two limiting cases of laminar and fully developed turbulent flows were treated and provided the maximum and minimum two-phase lengths respectively. The long lengths in the laminar flows are attributed to low viscosities associated with the low temperatures. The turbulent model, used in the present case, provides an eddy viscosity based strictly on dynamic quantities, that is, on the velocity difference between the axis and free stream. This accounts for the large,1000 to 1,ratio for the laminar to turbulent two phase lengths on the axis.

In TR 367 entitled "Finite Rate Evaporation of Cryogenic Hydrogen in Two Phase Air" by Edelman and Rosenbaum, (Reference 8) the restriction of equilibrium evaporation assumed in TR 349 was lifted, although the condensation of air was maintained as an equilibrium process. The rate relations involved in the evaporation of the hydrogen, was governed by two factors. The mass transfer factor from the particles was taken to be proportional to the difference in mass concentration of hydrogen at the particle surface and in the bulk gas phase, multiplied by a diffusion coefficient for mass transfer. Similarly, the heat transferred to the particle was proportional to the temperature difference. Calculations were carried out for a number of different initial conditions. Results are shown in corresponding curves for air initially in the gas phase. Figure 12 shows the particle radius R and the ratio of gas phase mass to the total mass. Figure 13, shows the hydrogen particle temperature and the gas phase temperature. Figure 14 and 15 show the gas phase and condensed phase mass fractions respectively. For all cases considered the evaporation time is of the order of 10^{-5} seconds for 1 micron particles.

In all of the foregoing summaries, we considered purely theoretical analytical results. An experimental program to investigate conditions for onset of ignition and combustion was also undertaken and was reported in GASL TR 404, entitled "Experimental Results for Thermal Ignition in Hydrogen in a Supersonic Viscous Flow" by J. Dunn. (Reference 9). This report presented the results of the study of hydrogen ignition in a turbulent boundary layer with particular reference to the effects of small protuberances in the flow. Tests were conducted in a combustion heated blowdown wind tunnel that exhausted to the atmosphere. The test section is shown schematically in Figure 16. Hydrogen was dumped into the test section through a wall slot, The wall slot was located in the fully expanded section of the wind tunnel and was three inches wide by 1/8 inch high. For all tests the total temperature of the hydrogen was approximately 580^{o}R. The splitter plate forming the boundary between the air flow and the hydrogen flow, had a thermocouple heliarced to the surface.

In addition to the flush wall test series, another series was run in which a 15^{o} half angle wedge was placed on the top wall of the test section (along which the hydrogen was vented). The wedge was located 9-1/4" (74 slot heights) downstream of the exit. The wedge was .45" high by 2-1/4" wide and did not span the test section because a wider span would choke the wind tunnel.

Another series of tests was run with a half cylindrical stainless steel rod welded to the splitter plate to assess the effect of local protuberances ½" upstream of the hydrogen slot on ignition characteristics. Two different rod sizes were used, one with a sixteenth inch radius and a second with a 3/16" radius. The rod length was 3½"(test section width).

Pressures, temperatures and heat transfer rates were measured during each of the above tests. Tests were performed under conditions such that the splitter plate wake alone was not sufficient to ignite hydrogen from the slot. Thus, air flowing from upstream at a static temperature of 1500°R was not hot enough to ignite the hydrogen in the absence of any other disturbance. For static temperatures of the order of 1900°R the hydrogen would however, have ignited.

It was concluded that:

1. Slot flow autoignition of hydrogen in air can be expected if the maximum temperature of the splitter plate boundary layer is 1900°R or higher. The temperature for autoignition is probably below 1900°R but is definitely above 1600°R, at the pressures in question (6 psia). The principal effect of static pressure would be to change the ignition delay and reaction times (lengths).
2. Thermal ignition of unburned hydrogen from a slot that is compressed by passing through a shock can be expected if the "unmixed" maximum splitter plate boundary layer temperature is raised to 1900°R by the shock. Alternatively, if the maximum temperature in a hydrogen air boundary layer is raised to 1900°R by passing through a shock thermal ,ignition can be expected.

3. A blunt proturberance ahead of the slot exhaust with a height equal to or greater than the boundary layer displacement thickness can generate enough hot gas to significantly alter the ignition characteristics of the slot flow. A temperature of 1900°R in the protuberance wake at the slot exhaust can be taken as the ignition temperature (at 6 psia).
4. The theoretical ignition delay curves appear to be in reasonable quantitative agreement with results from these tests and previous GASL work.
5. Heat transfer increases of 1.7 to 2.3 were measured during combustion in the constant area channel. Turbulent wall heat transfer rates in the reacting flow were observed to be 30% higher than would be predicted by using heat transfer relations developed for non-reacting flow and corrected for pressure as measured in the flow.

It is believed that this relatively small increase in heat transfer rate is attributable to the insulating effect of the hydrogen as noted in previous analytical studies.

As discussed above in TR #385 (Reference 5), there was developed an implicit finite difference procedure for the solution of the laminar boundary layer equations with chemical combustion. As noted the procedure worked very well for pure diffusion but did not work at all well when the finite rate chemistry became a factor of significance. Of crucial importance in this behavior was the fact that the chemical source terms were treated as known functions of the previous step because of their non-linear form (generally quadratic or cubic in the mass fractions). The resulting solutions resulted in oscillatory and negative mass fractions, when the step size exceeded certain very small values, except when the reaction rates were all set identically to zero. Iteration of the solution by recomputing the chemical sources in terms of last computed mass fractions, did not eliminate the generation of negative species. Indeed, the iteration at times exhibited its own characteristic type of instability. The reason for this highly unsatisfactory state of affairs became quite clear as a result of a detailed investigation by G. Moretti, Ref. 10 and D. Magnus on the one-dimensional flow of a reacting gas. These investigations showed that the calculations using Runge-Kutta and Predictor-Corrector techniques resulted in negatively damped oscillation of the trace species, particularly OH, when step size exceeded certain fixed values. Moretti showed further, that the same oscillations were developed by the system of chemical equations after linearizing the chemical source terms. It became clear that the oscillations were due to instability associated with the technique of integrating the chemical equations and were conceptually related to the kind of instability encountered in explicit solutions of partial differential equations. It was also clear that the linearization of the source terms made possible the application of new techniques for integrating the one dimensional chemical equations which could eliminate the problem of instability. In Reference 10, Moretti examined the exact solutions of the linearized equations, namely the exponential solutions. It was found that the allowable stepsize for accurate computation could be increased by several orders of magnitude. Subsequent investigations by DeGroat and Abbett established that a finite difference solution based on the subdomain technique, was stable, and was somewhat faster to solve on a digital computer than the exponential solution method which required determination of complex eigenvalues and a fairly involved succession of numerical steps. A summary of their techniques of solution and of the linearization is given in the Appendix of GASL TR 516 entitled "Laminar Boundary Layer Calculations with Finite Rate Chemistry", addendum to TR 385 by S. Slutsky and H. Rosenbaum. (Reference 11). This report describes the technique of incorporating the one-dimensional chemistry into the two-dimensional viscous flow field. As an example of the diffusion and chemistry system there was considered the case of a laminar boundary layer of hydrogen flowing in a uniform stream of hot air. The external air temperature was taken as $1000^{\circ}K$ at a pressure of one atmosphere. The temperature of the wall was assumed to be constant at $500^{\circ}K$. In Figure 17 there are shown boundary layer temperature profiles at various axial locations.

The initial temperature profile was chosen to correspond to a Crocco integral. As the hot air stream mixes with the hydrogen boundary layer combustion occurs and,as can be seen from the temperature profile,the combustion zone is quite narrow compared to the boundary layer thickness, suggesting the applicability of a flame sheet model. The associated species mass fraction profiles at three representative axial stations are shown in Figures 18, 19 and 20. Figure 18 shows the initial profiles, Figure 19 shows the profiles at 2.55 feet and Figure 20 at 8,56 ft. Notice in Figures 19 and 20 the narrow region in which the water concentration peaks, the oxygen concentration diminishes and which also corresponds to the region where the temperature peaks. This flame sheet region is narrow in extent compared to the boundary layer since characteristic reaction times for hydrogen combustion are much smaller than the characteristic times associated with laminar diffusion. The simple flame sheet models, References 2 and 4, assume that hydrogen and oxygen are annihilated in the flame sheet and that there exists no oxygen in the hydrogen rich region. In the more realistic model of TR 516 oxygen is mixed with the hydrogen due to diffusion prior to the combustion initiation as seen in Figure 19 and 20. After combustion begins the oxygen diffuses into the flame region from both sides of the high temperature region. The physical situation treated in this calculation, is one wherein excess hydrogen is dumped from the vehicle adjacent to the vehicle surface. The possibility of ignition of this hydrogen depends on the presence of an upstream disturbance such as a shock which provides a high temperature air flow in the vicinity of the jet. In this case the calculation shows that for a distance on the order of 10 feet, which is long compared to the distance for transition to turbulent flow under normal flight conditions, the flame or region of high temperature is kept well away from the vehicle wall.

In TR 425 entitled "Multicomponent-Multiphase Viscous Flow with Chemical Reactions", Part I, Analysis, by R. Edelman, Ref. 12 there was developed a physical model and computational scheme for the study of viscous jet mixing configurations in the presence of condensed phases. In TR 508 entitled "Multicomponent-Multiphase Viscous Flow with Chemical Reactions" Part II Computations, by R. Edelman and G. Weilerstein, Reference 13, the computational scheme was extended to include the additional capability required for treatment of chemically active jet flows. In addition, numerical computations were carried out for both chemically active and frozen flows.

The basic configuration of the flow field is shown in Figure 21. The jet is an axisymmetric, fully expanded stream of low temperature hydrogen and the outer flow is a uniform stream of moist air. The jet temperature is sufficiently low to condense the O_2, N_2 and H_2O after mixing has occurred. The free stream temperatures were chosen below and above the ignition limit to provide conditions for chemically frozen and active two phase flows. The latter is the more general case and leads to a flow field as depicted in Figure 21. Region A represents the core of pure hydrogen which is virtually unaffected by the diffusion process. In region B mixing has occurred but the temperature levels are well below the required temperature for ignition. This region is predominantly H_2, 0_2 and H_20 in two-phase states with only traces of gaseous 0, H and 0H. Region C represents a zone of intermediate temperature levels which are above those required for two phase states and not yet high enough for ignition. Combustion takes place at the higher temperatures which prevail in Region D where significant concentrations of all seven species appear. The approach to the free stream state is accompanied by the disappearance of hydrogen and combustion subsides. Therefore, region E is a zone where mixing has occurred without significant chemical activity.

Figures 22a, b, and c, show the radial distribution of the pertinent variables associated with the low temperature, chemically frozen case at a representative streamwise station. The hydrogen jet is all gas at 40°K and the free stream is at a pressure corresponding to an altitude of 40KM (6.3 lb/ft^2) and a temperature of 260°K.

Figure 22a, shows the mixture mass fractions for the four components present in the low temperature flow field. The non-monotonic distribution of the H_20 is of particular interest since this behavior is a result of the phase separation phenomenon. As the flow field develops the H_20 gas diffuses inward and is cooled sufficiently to condense. The condensed fraction undergoes no further diffusion and merely flows along the streamlines described by the local mean gas phase velocity. A zone of condensate is developed as additional H_20 vapor is condensed on adjacent streamlines. Closer to the axis the N_2 and 0_2 begin condensing and form a less pronounced condensed phase zone illustreated in Figure 22b.

To study the behavior of a two-phase system with combustion the free stream temperature and pressure were increased to 1500°K and 114 lb/ft^2, respectively. The pressure corresponds to an altitude of 20KM where the hydrogen jet at the temperature of 40°K is in an all gas state. Radial distributions of the pertinent variables are shown in Figures 23 which represents the flow field configuration at a streamwise station where significant chemical and two phase phenomenon are present. Figure 23a shows the mass fraction distributions of the four major components in the flow field. The appearance of significant chemical reaction is evident by the large increase in the mass fraction of H_20 in the high temperature region ($900<1500^{\circ}K$). Additional evidence of combustion in this region is the depletion of 0_2 and H_2. The corresponding mass fractions of 0, H and 0H attain their peak values within this combustion zone as shown in Figure 23b.

The nature of the above results are in part governed by the model assumption regarding transport phenomena in this two-phase system. The assumption that viscous transport is a gas-phase process requires justification particularly in turbulent flow fields. If the particles are small (low micron to sub-micron range) and in addition small compared to the microscale of the gas-phase turbulence, the particles will follow the gas-phase motion. Under these conditions, turbulent transport in the particulate phase can be expressed in terms of an eddy viscosity equal to that of the gas-phase. If the particles are large compared to the microscale of the gas-phase turbulence the particulate phase eddy viscosity will be small compared to that of the gas-phase and the particles will not diffuse but will be governed by the <u>mean</u> gas-phase motion. The calculations presented here simulated gas-phase turbulence with a viscosity one hundred times the local laminar value. If the particles were allowed to diffuse in accordance with the "small particle" conditions described above, there would not have resulted the "pop" in the H_2O mixture mass fraction distribution. The tendency to accumulate would vanish in the regions where condensed phases exist.

In essence then, the capability to treat combined combustion and two-phase configurations in laminar and turbulent flows is considered to have been generated. The possibility of a simultaneous plume of water and of hydrogen combustion in the region behind a strong shock was considered.

In the aforementioned studies no attempt was made to treat the effect of turbulence along the vehicle boundary layer. Such an effect can be of importance in the evaluation of alternative modes of hydrogen ejection. For example, if the hydrogen is dumped overboard via a tube oriented parallel to the vehicle surface and some arbitrary distance away from it, the possibility exists of hydrogen diffusion into the wall boundary layer. At supersonic speeds the wall boundary layer contains high static temperatures and if sufficient hydrogen diffuses into this region the danger of combustion arises.

To analyze such problems a turbulent boundary layer analysis was undertaken and is reported in GASL TR 514, entitled "Compressible Turbulent Boundary Layer with Application to Hydrogen Dumping and Combustion" by H. Rosenbaum, Reference 14. In order to pursue this investigation it was first necessary to formulate a model for the turbulent boundary layer. Once this model had been formulated and tested the hydrogen dumping problem was considered as an application.

The basis of the analysis is two-fold: application is made of transformation theory to reduce the velocity field in a compressible flow to that corresponding to an incompressible constant property flow and adequate description was provided of the velocity field corresponding to that in an incompressible turbulent boundary layer. The recent work of Coles and Crocco has made available a general transformation for turbulent flow which requires no specification of arbitrary reference states as did earlier informations.

For the purpose of justifying the formulation and finite difference solution technique of the energy conservation equation, an incompressible heat transfer calculation was performed and compared to an experiment for various effective Prandtl numbers. These results are shown in Figure 24 to 25. Then a compressible flow calculation was performed to determine the skin friction distributio on an adiabatic wall in a Mach No. = 2.7 flow. The comparison of this with the experiments of Matting and Chapman are shown in Figure 26.

A calculation, including the effects of finite rate chemistry, corresponding to an air boundary layer with a hydrogen exterior was next performed. As the hydrogen diffuses towards the wall its temperature, due to the high wall temperature, will increase and combustion can be initiated. This approximates the physical situation wherein hydrogen is dumped overboard in the vicinity of the vehicle boundary layer. In Figure 27 there are shown the initial profiles of temperature ratio and species mass fractions. Figure 28 shows the wall concentrations downstream of the initial region. Figure 29 shows the distributions of species mass fractions at the axial station where the calculation was terminated. Figure 30 shows the corresponding temperature profile. Although no significant temperature rise in the boundary layer has occurred it is evident from the reaction products present that combustion had begun. The calculation implies that extreme care must be exercised in the dumping of the hydrogen in order to avoid the possibility of combustion.

An experimental study of diffusion of hydrogen from a jet of radius "a" into the turbulent boundary layer and of subsequent combustion was considered. The first phase of the program which was designed to investigate the diffusion from the jet into the boundary layer is reported in TR 525 entitled "Experimental Studies of the Diffusion of a Light Gas Exhausting into a Supersonic Air Stream in the Vicinity of a Wall" by J. Tamagno and M. Recarey, Reference 15.

Qualitative analytical predictions of the three-dimensional flow pattern which develops in the mixing region between the injected gas and the primary flow were obtained using a linearized technique which reduces the species conservation equation to one formally identical to the classical unsteady heat diffusion equation. Also a two-dimensional turbulent boundary layer analysis was used to give an approximate, but conservative extrapolation of wall concentration further downstream of the region investigated experimentally.

The experimental investigation was carried out using a turbulent jet of helium exhausting into an air stream at a distance D from the wall .

Tests were performed at two relative distances a/D of the tube from the wall.

1. The injection tube located at a/D=1.7
2. The injection tube located at a/D=3.

Measurements of static pressure, pitot pressure and concentrations were obtained at various stations downstream of the injection point. It was concluded from the investigation that the amount of an injected reacting gas which will diffuse into high temperature regions of the wall boundary layer may be kept below a dangerous point by simply locating the injector a few nozzle diameters above the wall (in the cases considered it was only required to have $a/D > 3$); on the other hand lowering the injector could result in sufficient accumulation of injectant into the wall boundary layer to initiate and sustain combustion.

III. CONCLUSION AND RECOMMENDATIONS

The fluid mechanical analyses have shown that the hydrogen and air will mix in lengths which are short compared to practical vehicle dimensions and form mixtures whose composition is such as to fall within the combustion limits of the air-hydrogen system. However, with perfectly expanded nozzles and no local disturbances, temperatures and pressures are such that combustion will not occur. If there are local hot zones in the flow field, combustion can be initiated, and once initiated will be maintained. One such hot spot investigated in detail here is the high static temperature region occurring in the boundary layer of the vehicle. Thus, if hydrogen is ejected in such a manner as to diffuse into the air boundary layer along the surface, combustion is predicted. It does not follow that hydrogen ejected within the boundary layer will burn immediately. The normal high static temperature peak appearing in an air boundary layer under supersonic flight conditions is suppressed because of the high heat capacity of the hydrogen. Here combustion can occur only after sufficient hydrogen has diffused away from the vehicle wall. These lengths may be long compared to vehicle dimensions. Despite this seeming advantage, ignition can still be induced in this configuration as a result of protuberances or irregularities in the vehicle surface or ejection hardware, as was observed in the experimental studies considered in the foregoing.

It appears that upstream ejection of hydrogen can be accomplished without hazard of ignition or combustion by venting via a parallel perfectly expanded nozzle. This should be displaced far enough from the vehicle to reduce hydrogen levels to below flammability limits.

It should be noted that the effect of nozzle underexpansion on combustion initiation was not treated in the foregoing studies. Nor were effects of pressure interaction with viscous jet mixing and chemical combustion or of more realistic treatments of turbulent transports. It is recommended that these effects be given further consideration because of their importance in the combustion and diffusion mechanisms appearing in a number of external flow problems of current interest and importance.

IV. REFERENCES

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15. Tamagno, J., and Recarey, M., "Experimental Studies of the Diffusion of a Light Gas Exhausting into a Supersonic Air Stream in the Vicinity of a Wall", GASL Technical Report No. 525, April 1965.

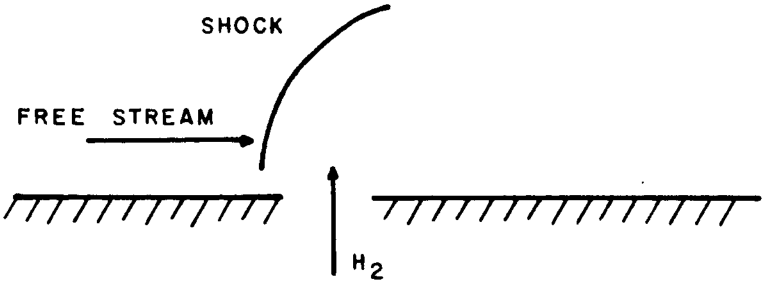


FIG 1(a) NORMAL INJECTION

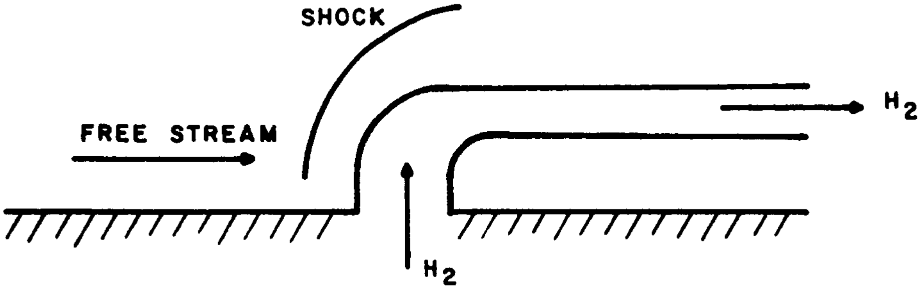


FIG.1(b) INJECTION THROUGH A TUBE

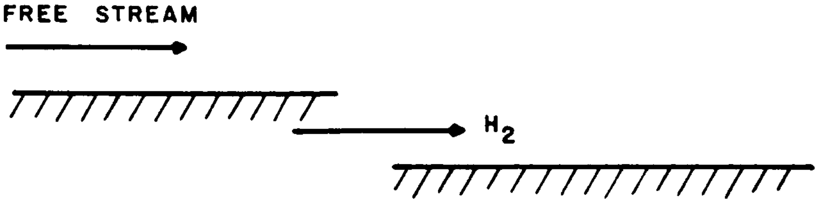


FIG. 1(c) SLOT INJECTION

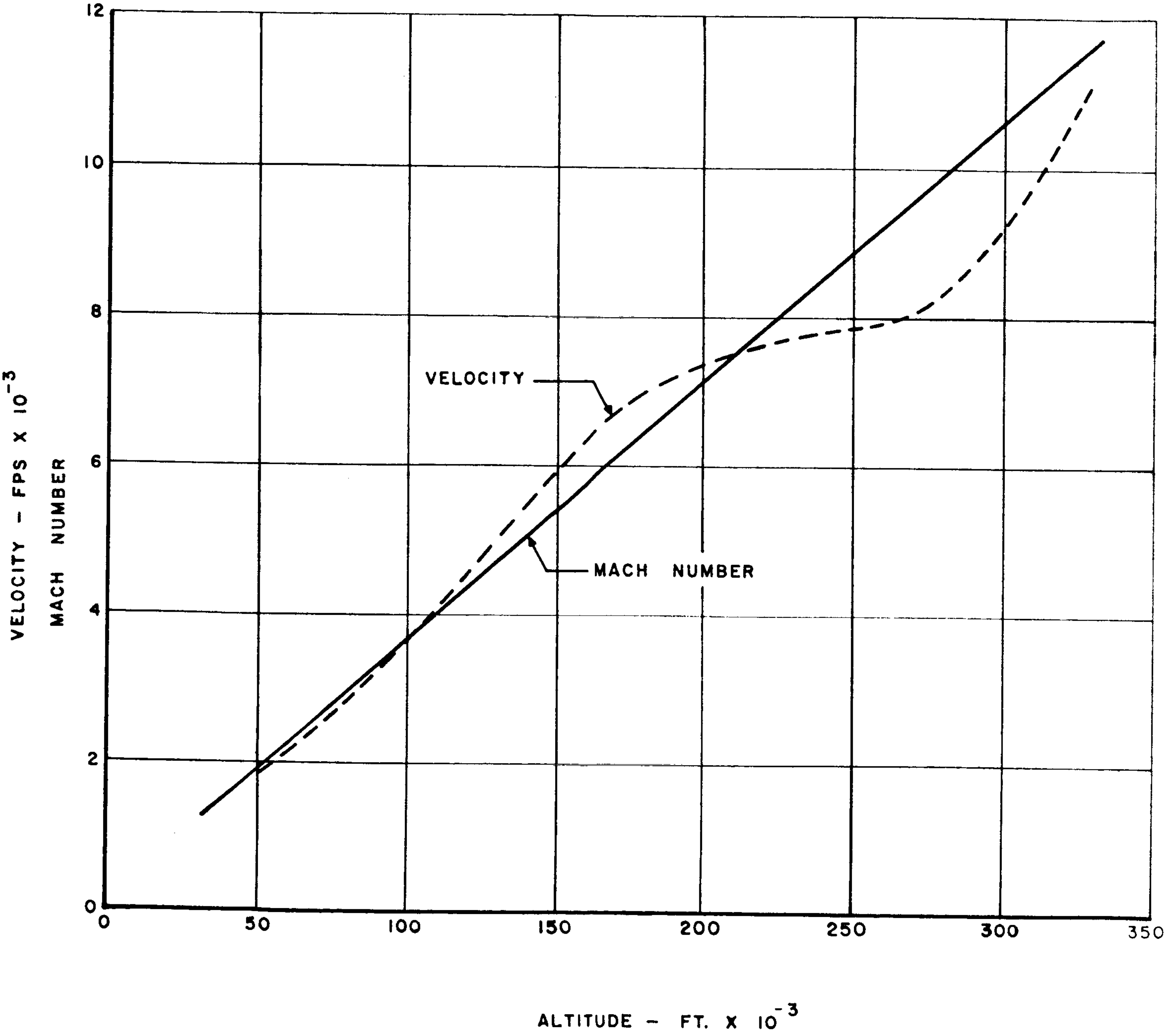


FIG. 2 FLIGHT CONDITIONS FOR LAUNCH TRAJECTORY

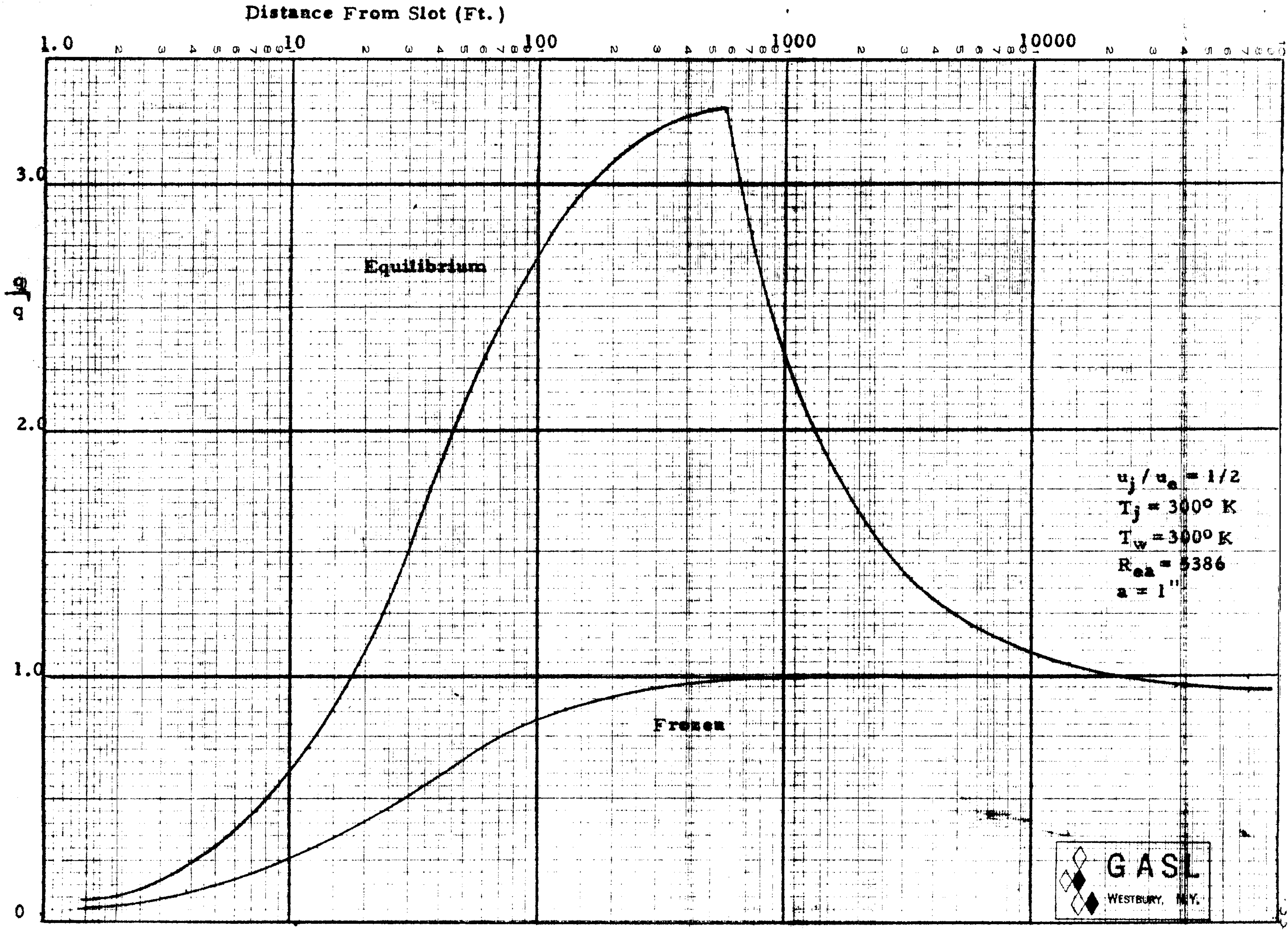


Figure 3 Heat Transfer Ratio

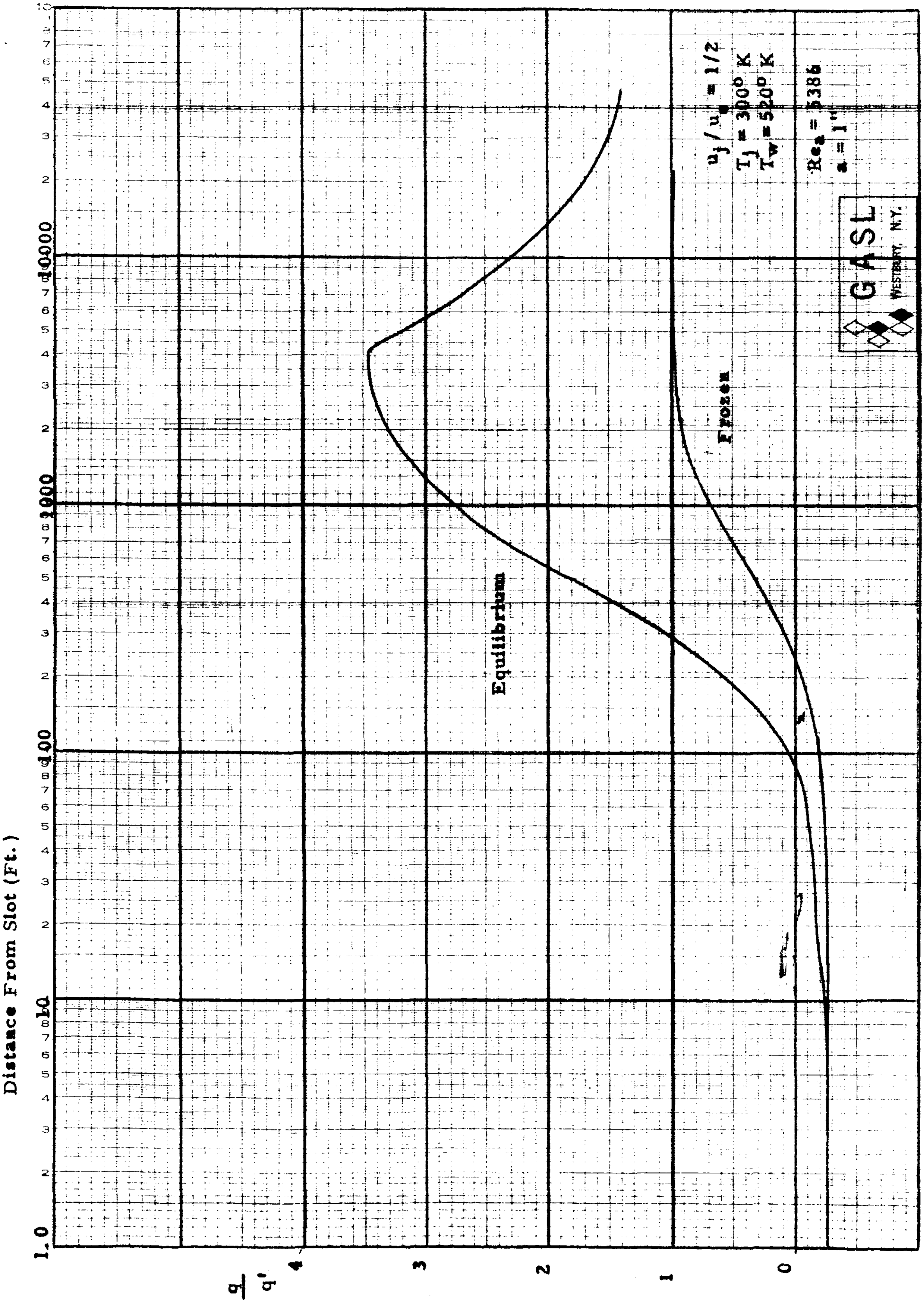


Figure 4 Heat Transfer Ratio

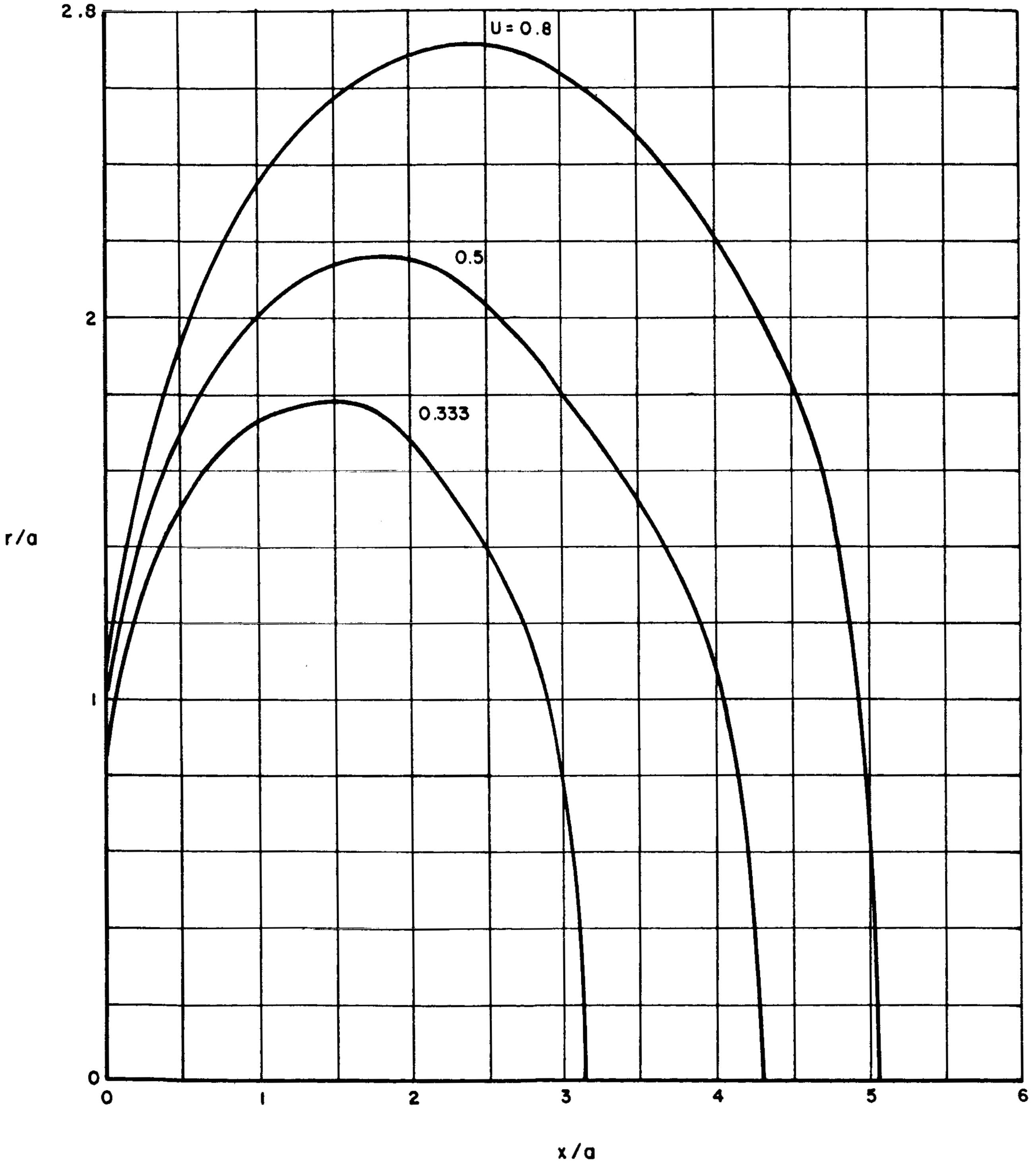


FIG. 5 TURBULENT FLAME SHEETS T_j = 265°K

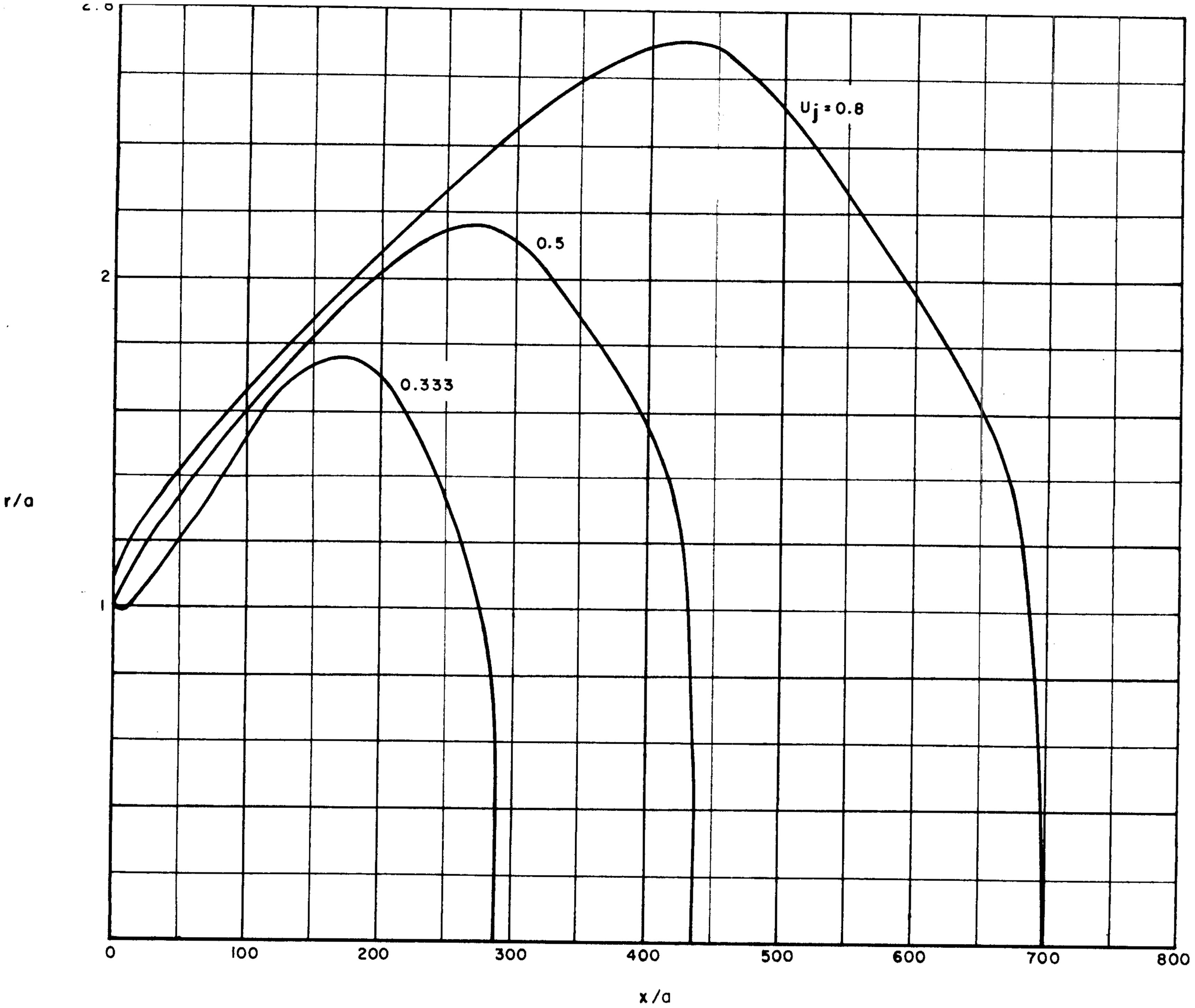


FIG. 6 LAMINAR FLAME SHEETS $T_j = 265°K$

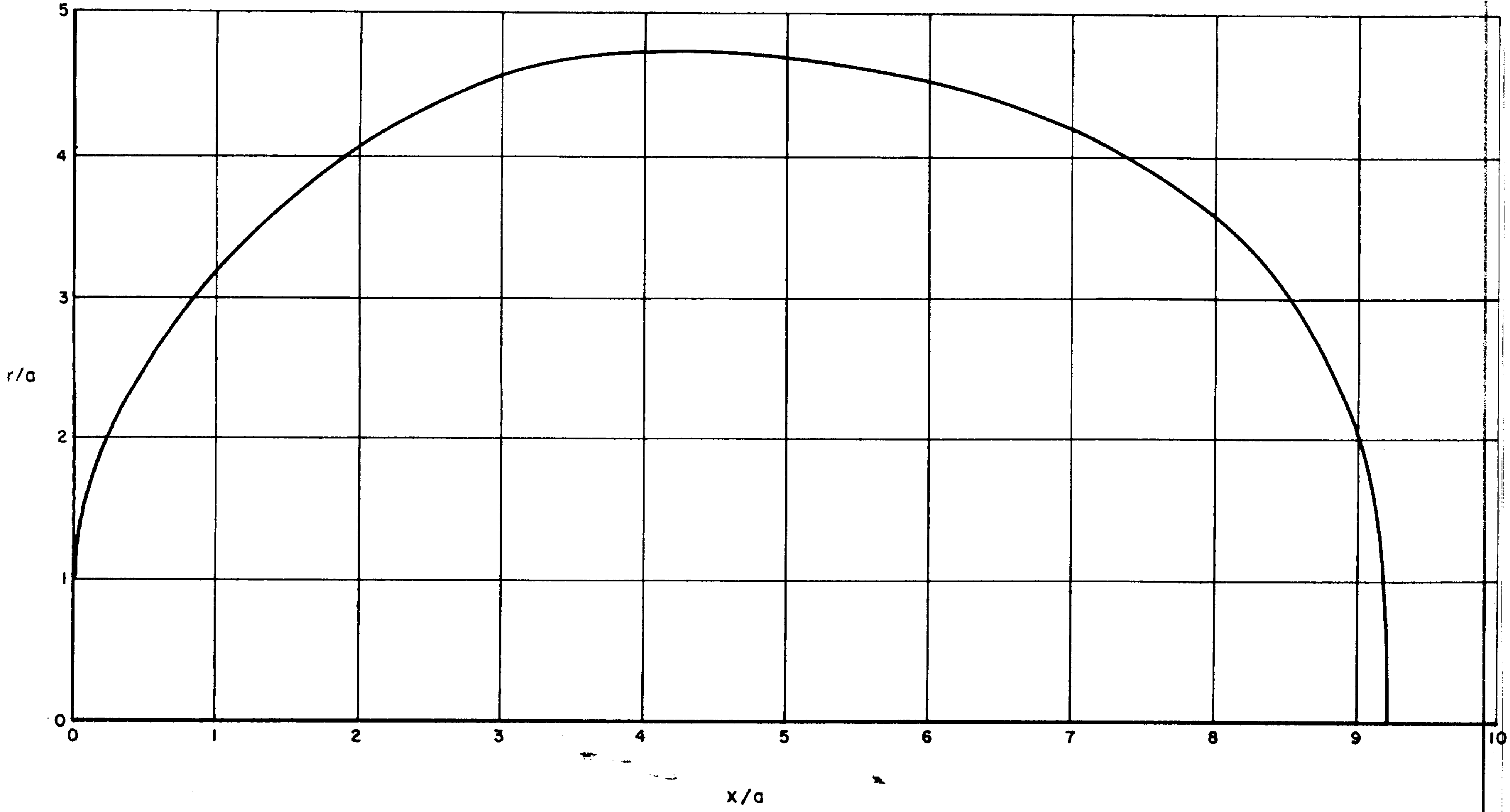


FIG. 7 TURBULENT FLAME SHEET - $T_j = 60°$ K

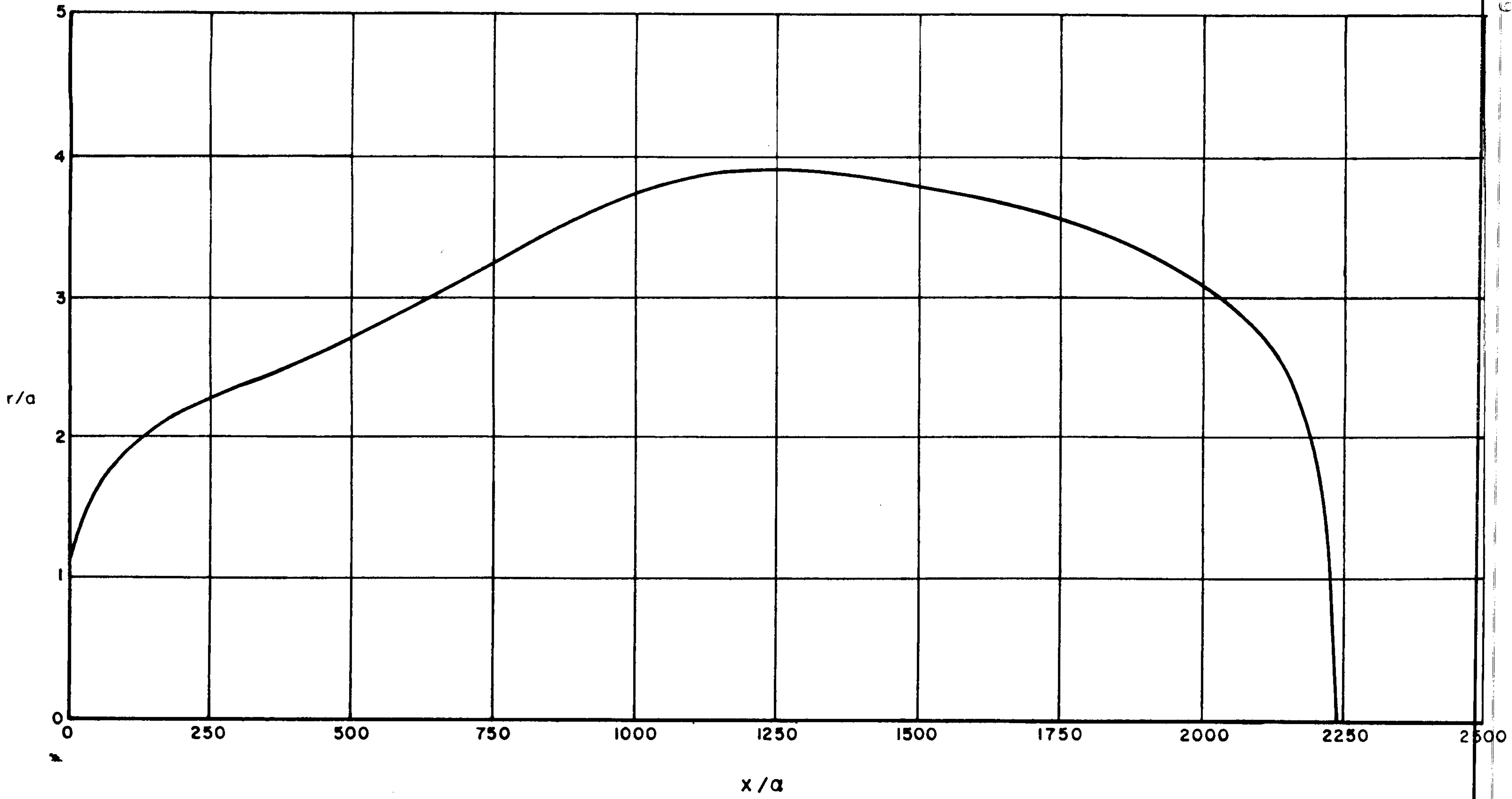


FIG. 8 LAMINAR JET $T_j = 60°K$

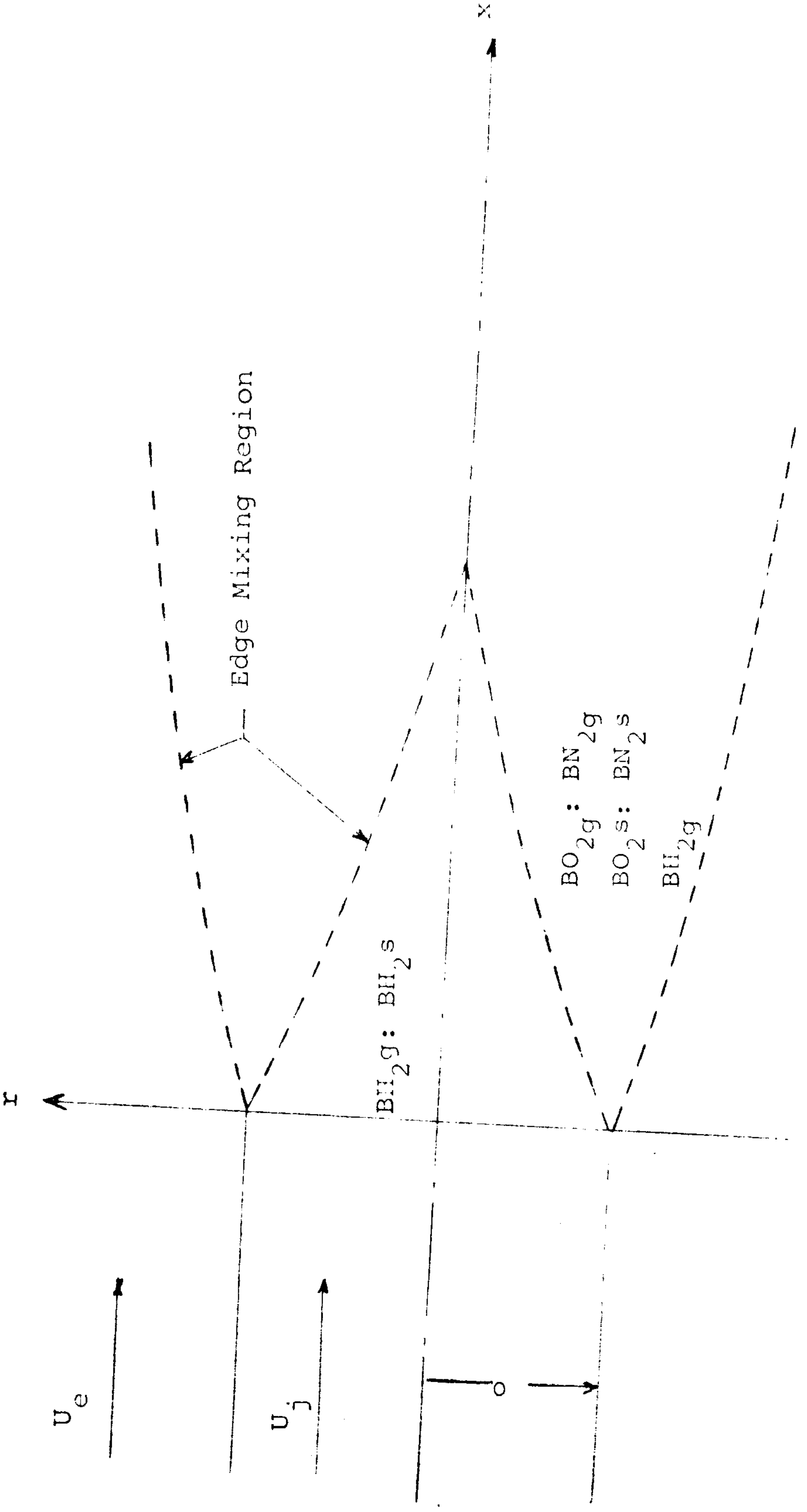


Fig. 9 SCHEMATIC OF FLOW REGION

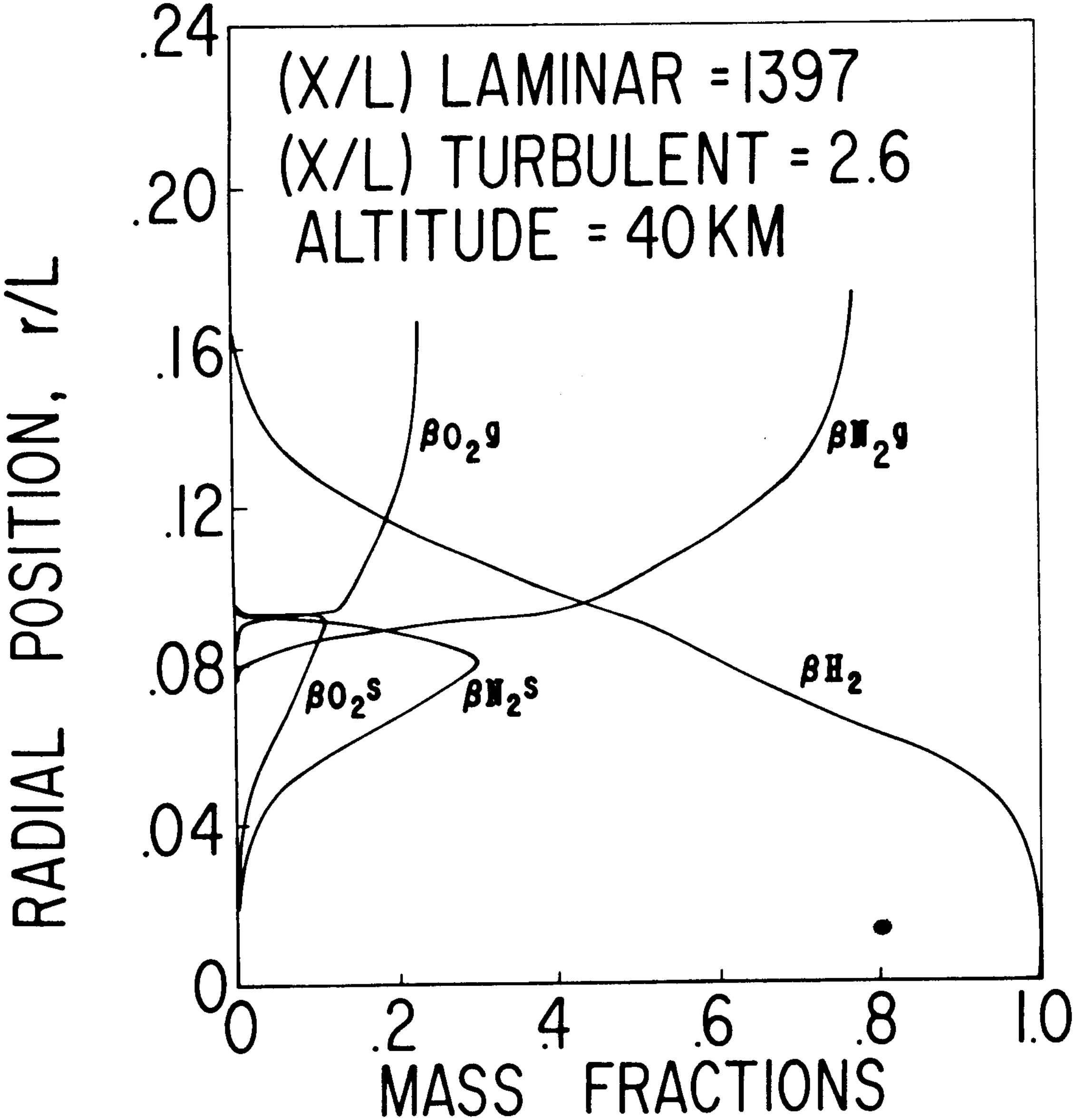


FIG. 10 RADIAL DISTRIBUTIONS OF CONDENSED PHASE AND GAS PHASE MASS FRACTIONS

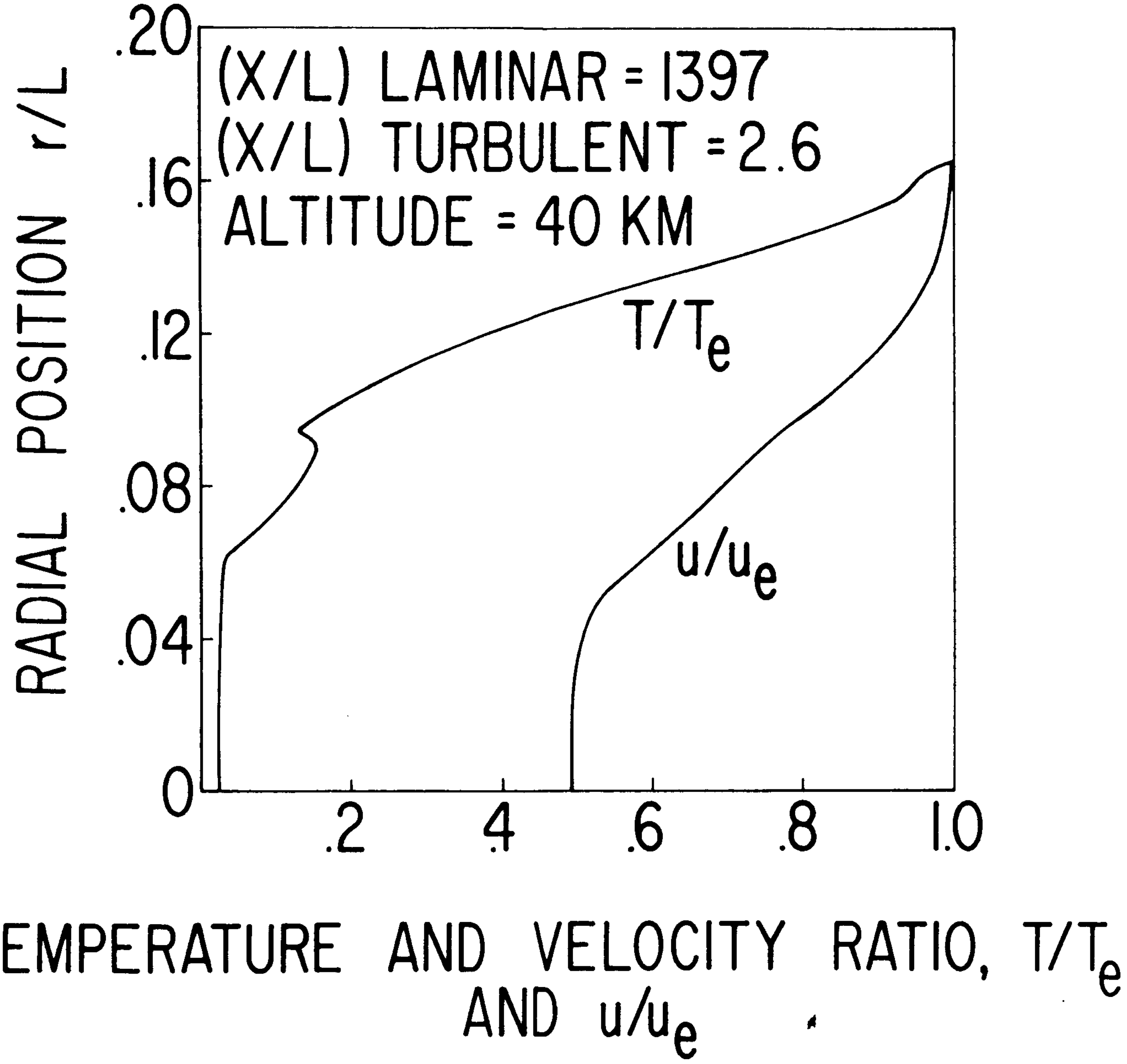


FIG. 11 RADIAL DISTRIBUTION OF VELOCITY AND TEMPERATURE

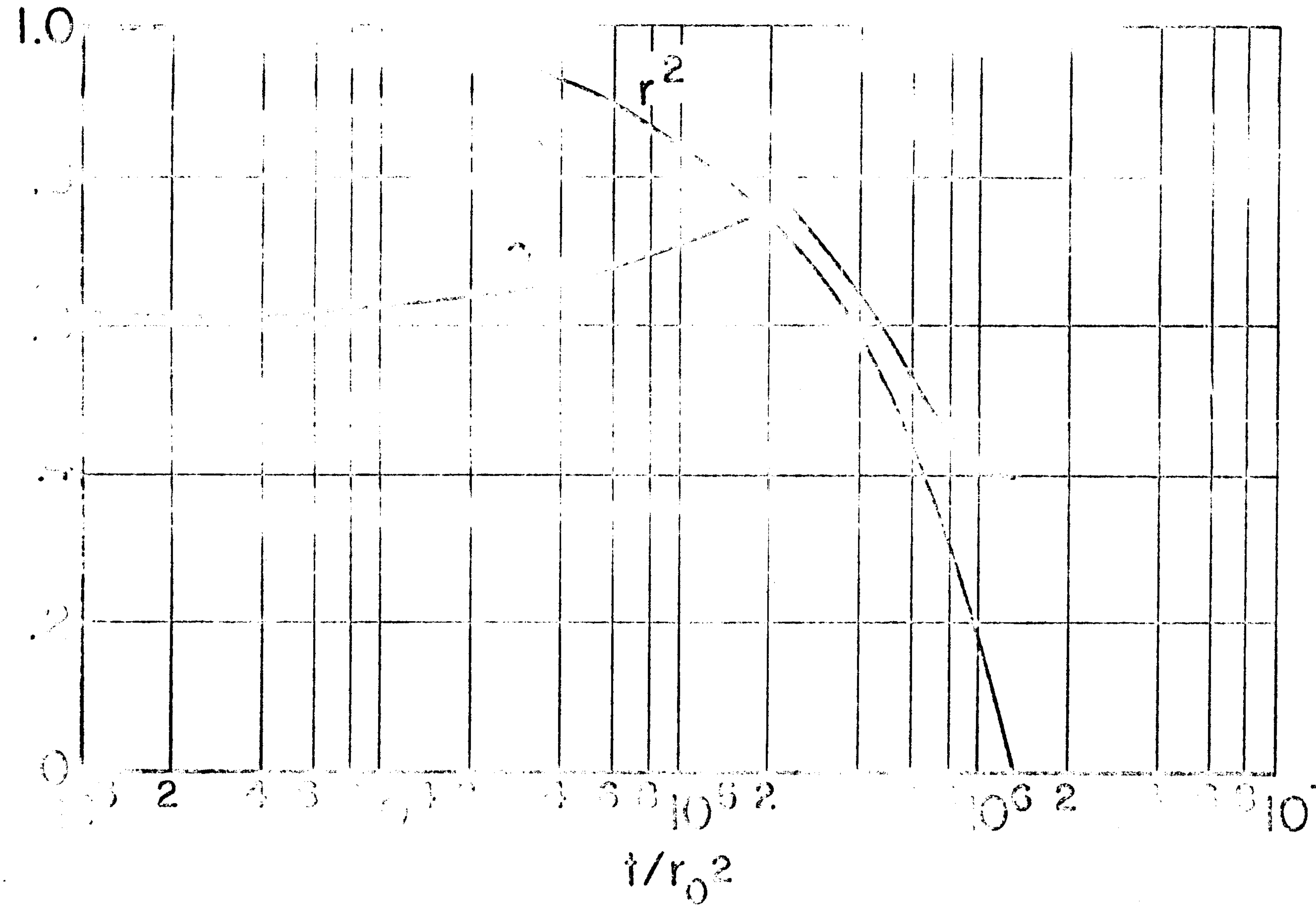
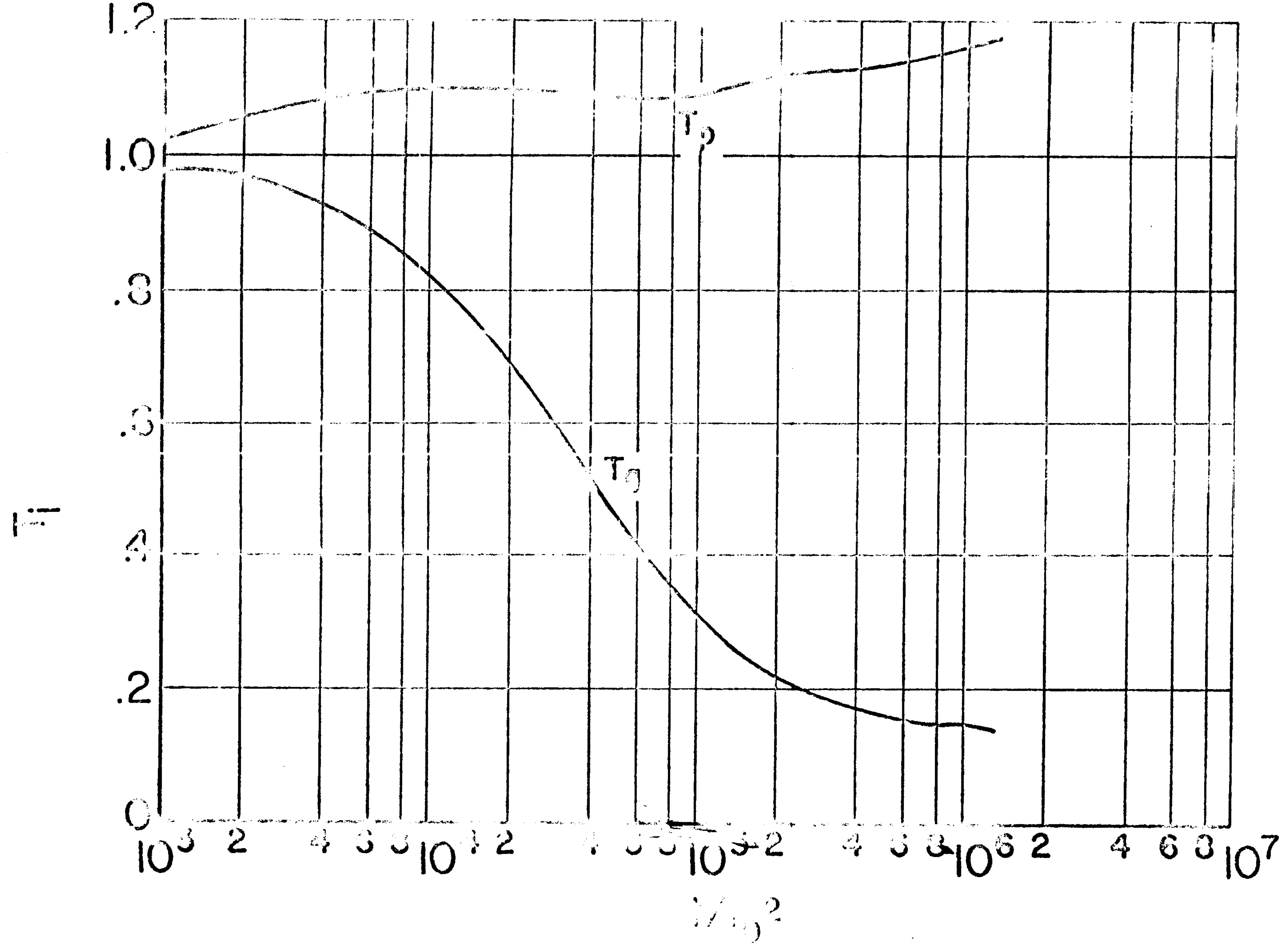


FIG. 12 PARTICLE RADIUS AND DEGREE OF VAPORIZATION VS. t/r_o^2



[illegible] 13 PARTICLE [illegible] RES VS. $1/r_0^2$

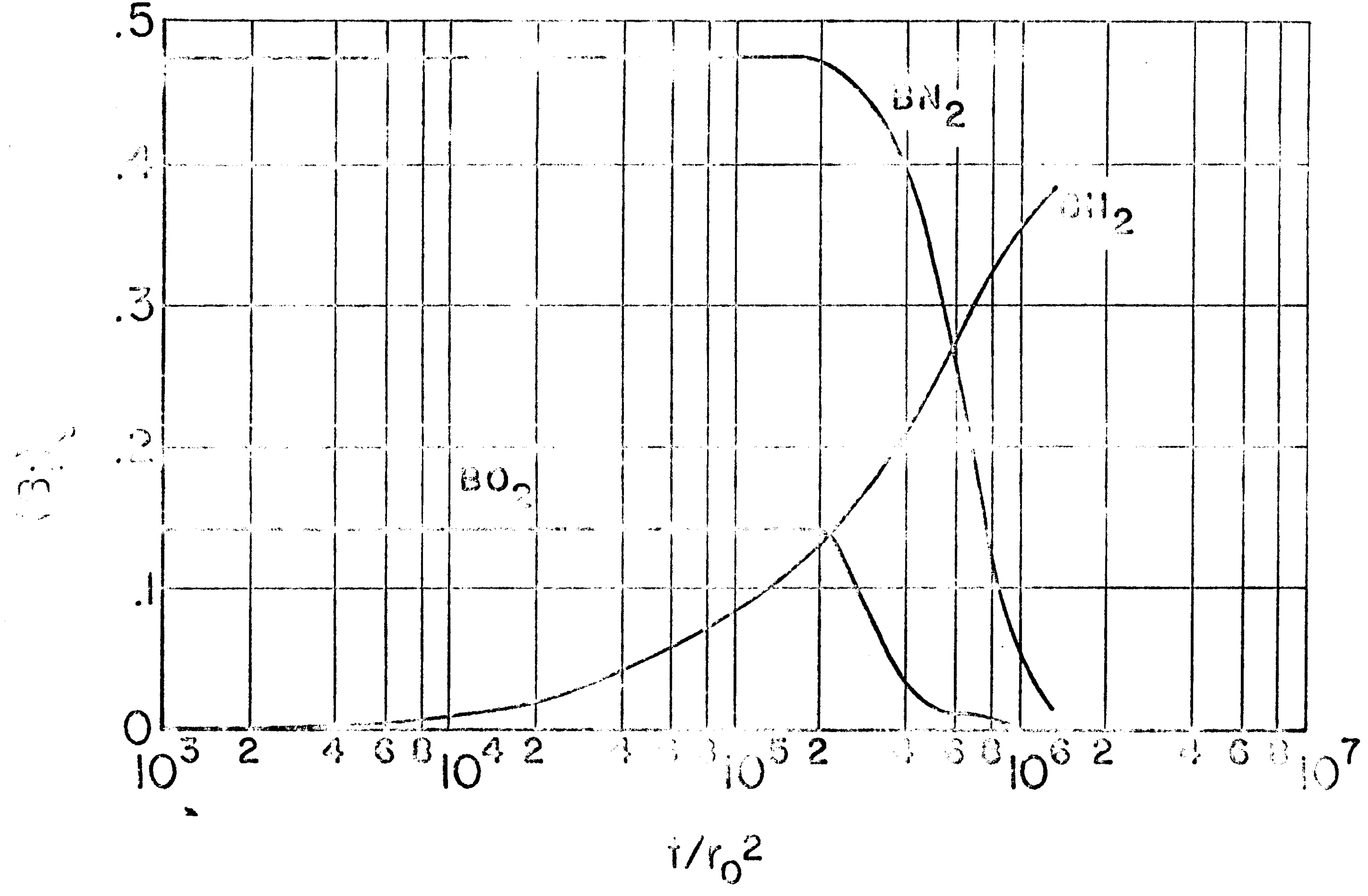


FIG. 14 GAS PHASE MASS FRACTION VS t/r_o^2

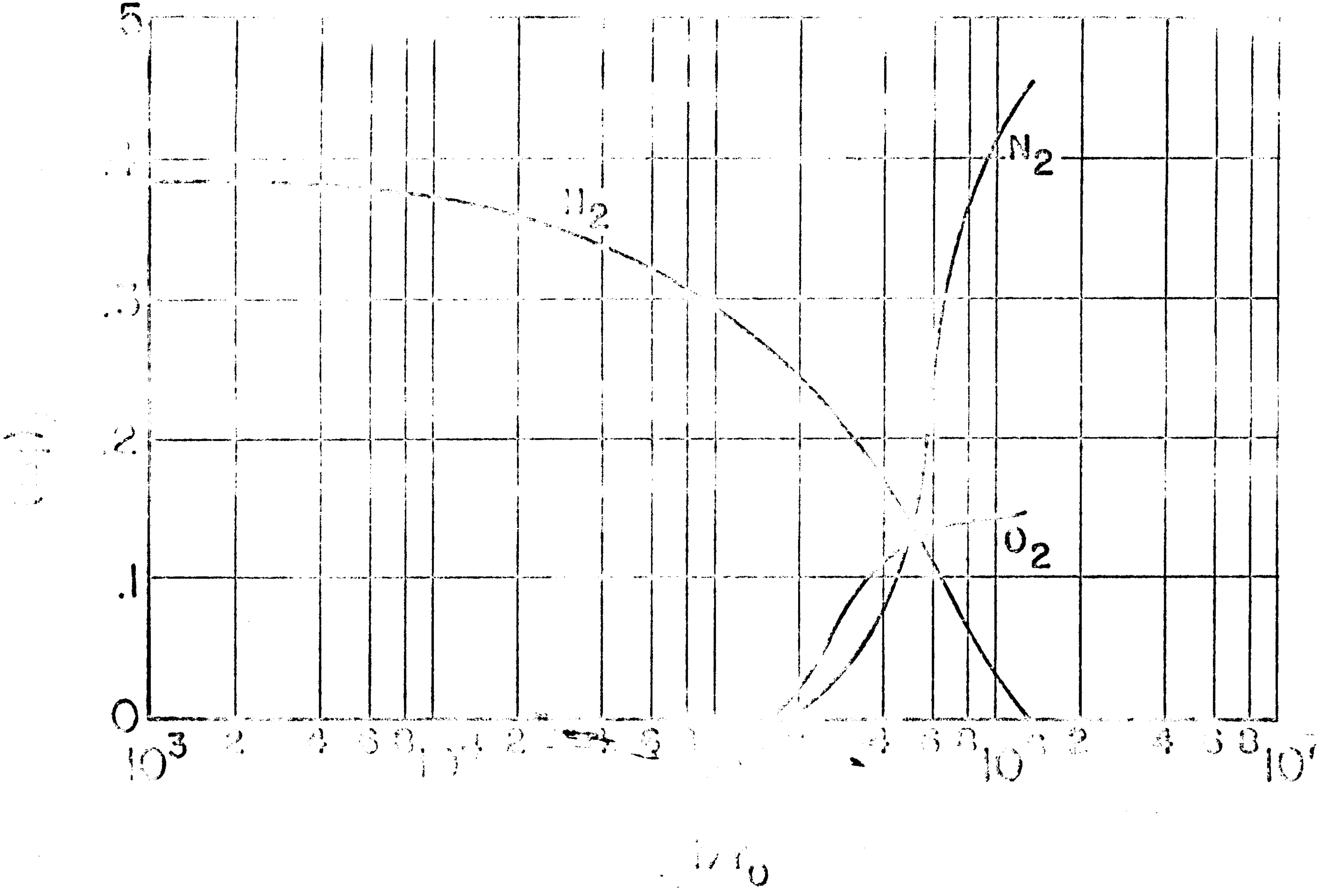


FIG. 15 CONDENSED PHASE MASS FRACTION VS. $1/r_o^2$

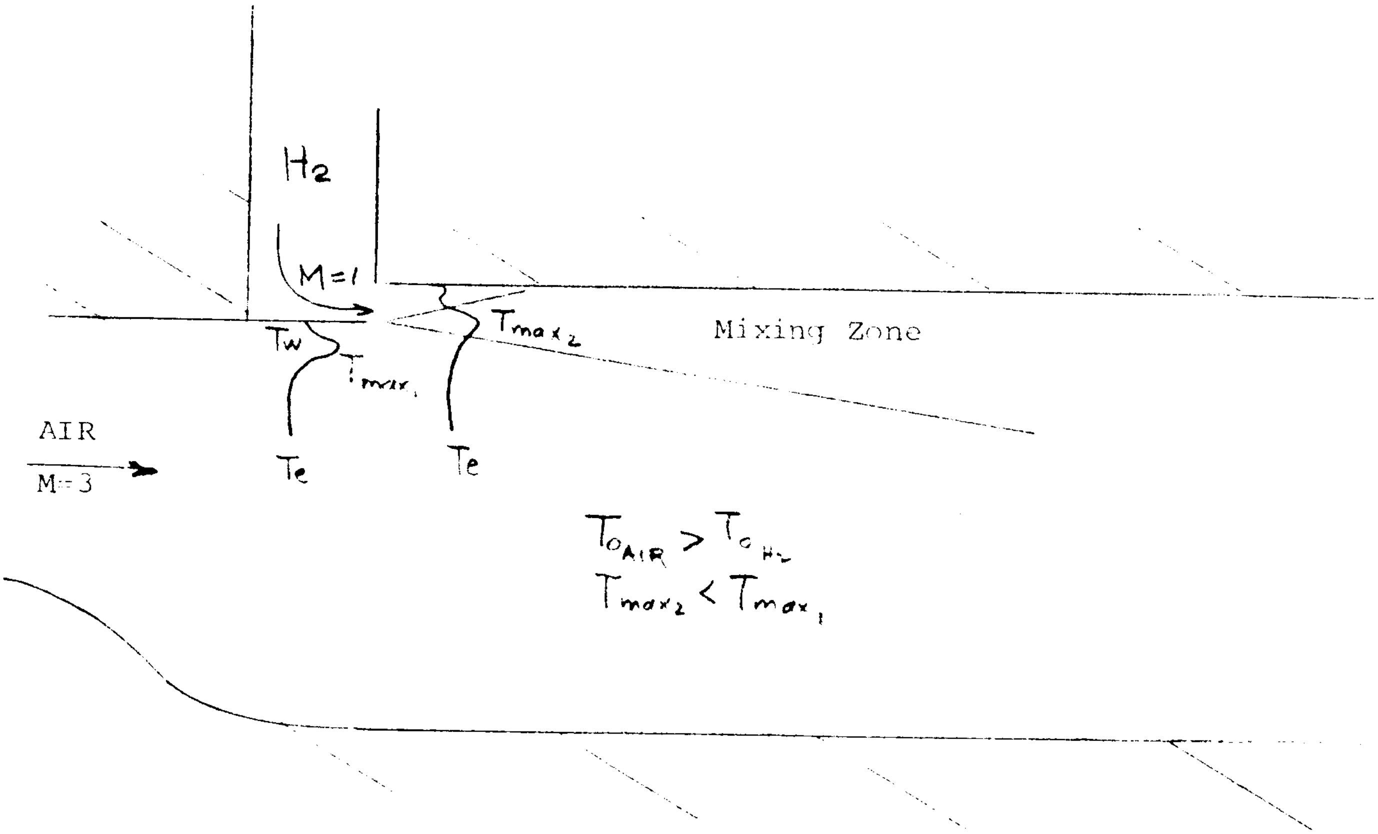


FIGURE 16

Schematic Representation of Temperature Profiles for Slot Mixing In Vicinity of Splitter Plate

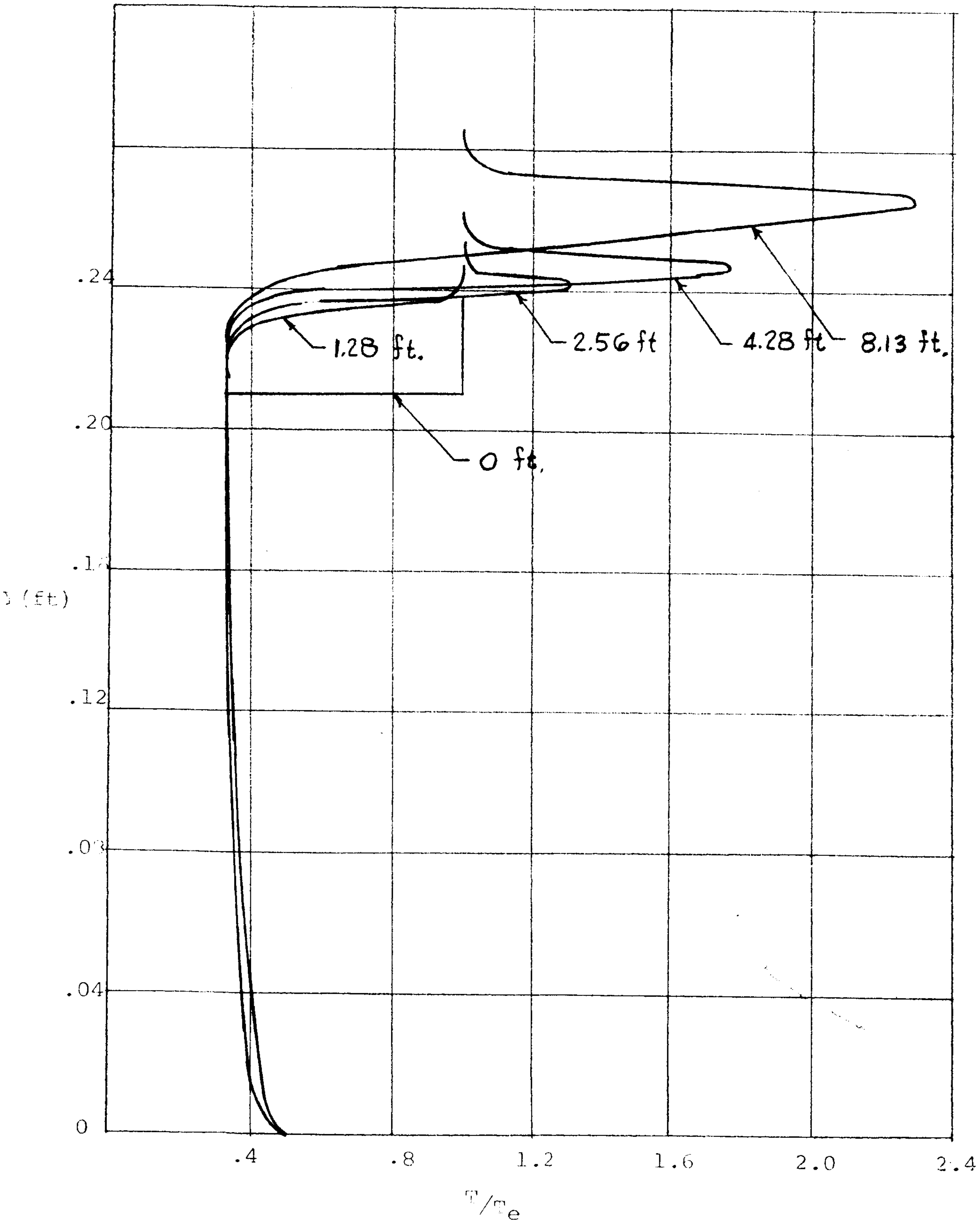


Figure 17 - Radial Temperature Distributions

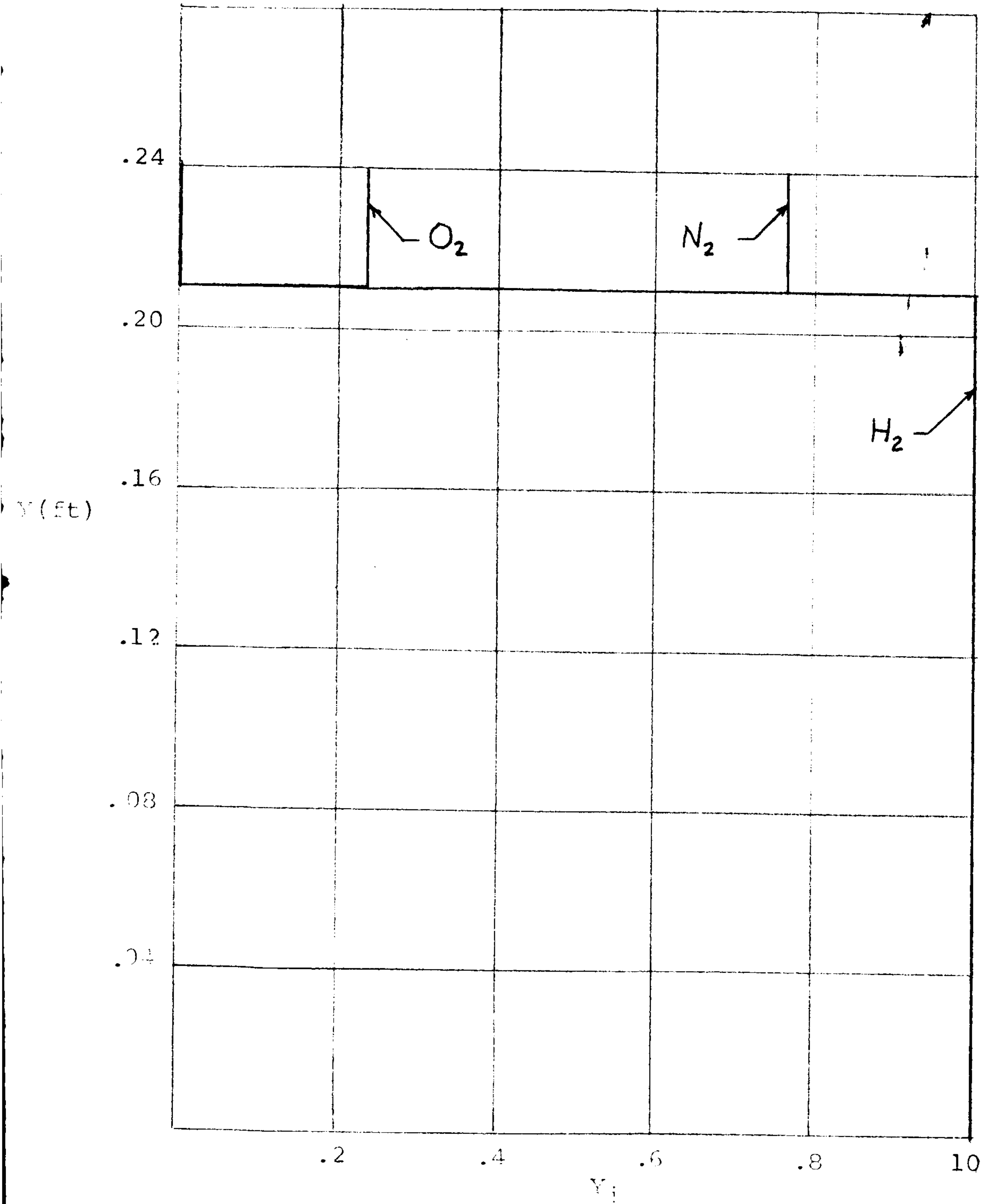


Figure 18 - Radial Mass Fraction Distribution, x = 0

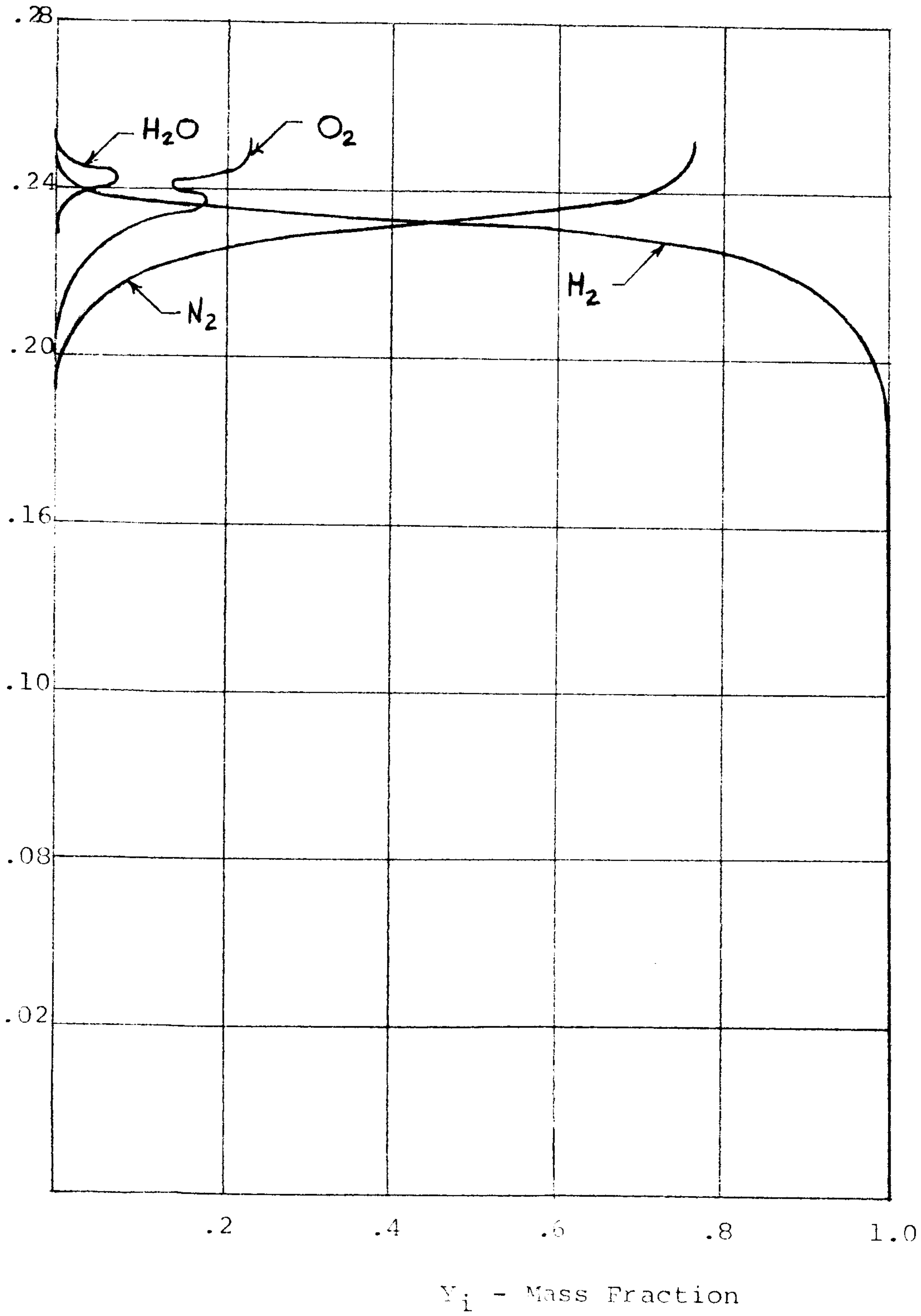


Figure 19 Radial Mass Fraction Distribution x = 2.56

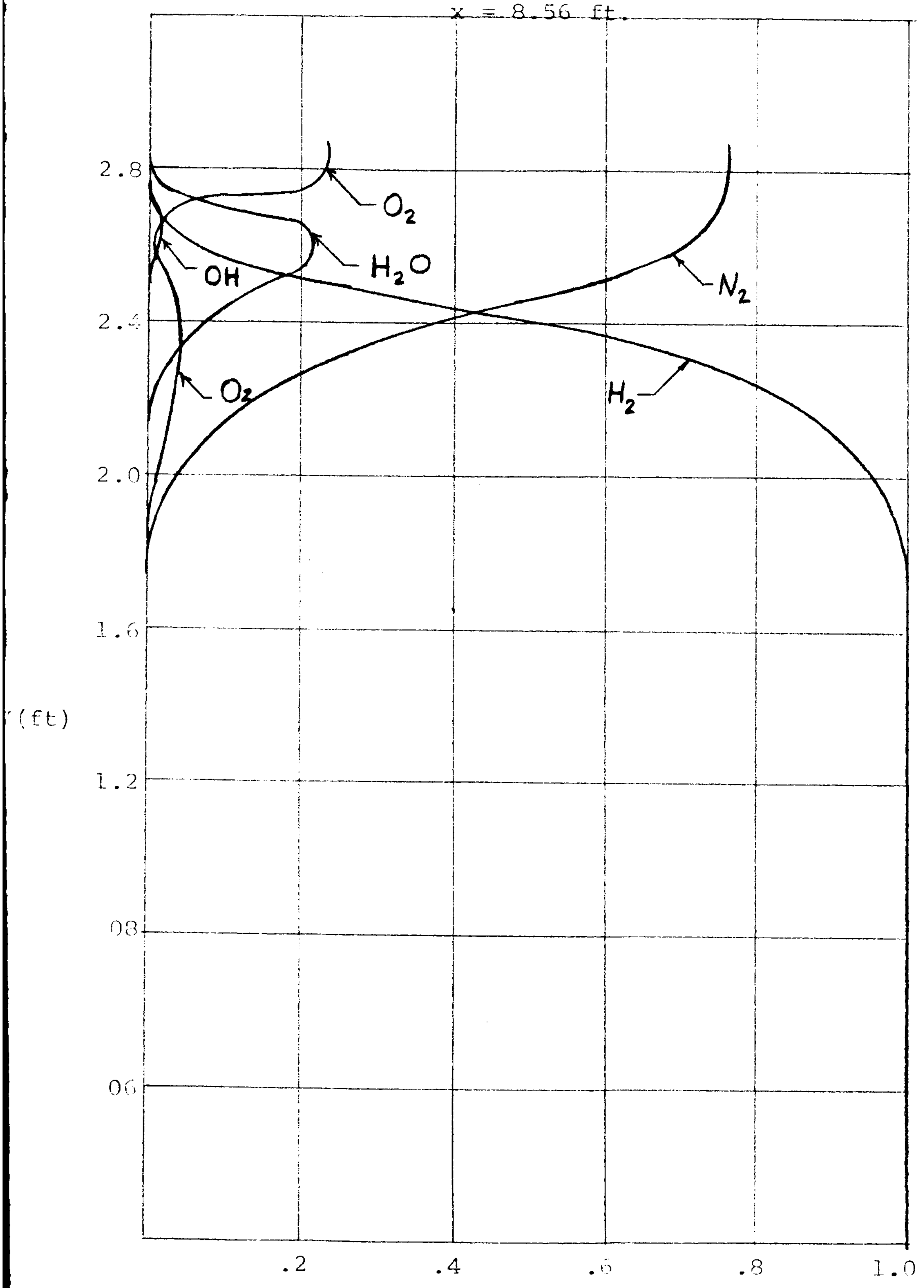
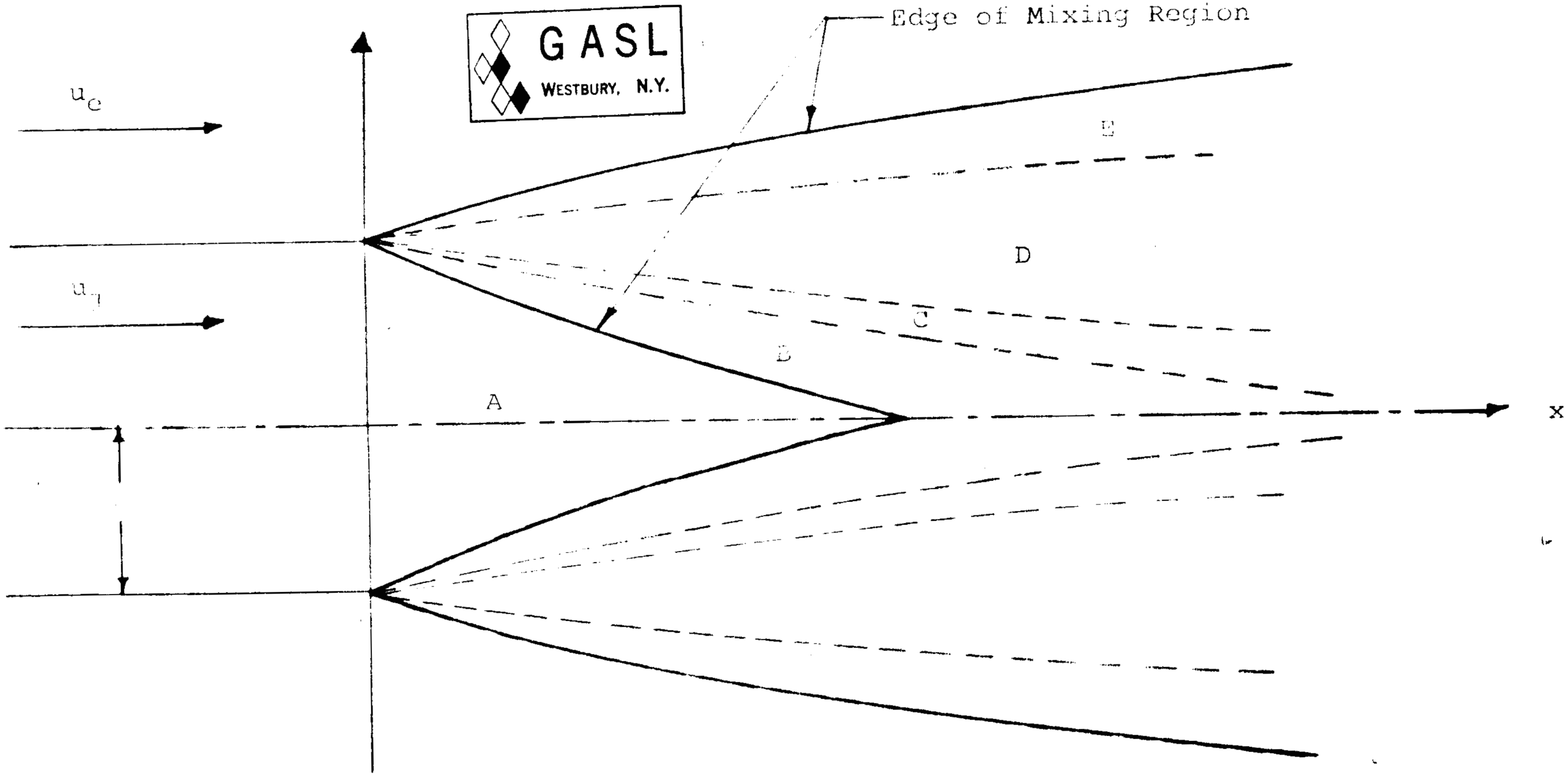


Fig. 20 Radial Mass Fraction Distribution, x = 8.56 ft.



A = Hydrogen core
B = Two phase mixture
C = Low temperature gas mixture
D = High temperature gas mixture with chemistry
E = Gas

FIGURE 21- SCHEMATIC OF FLOW REGION

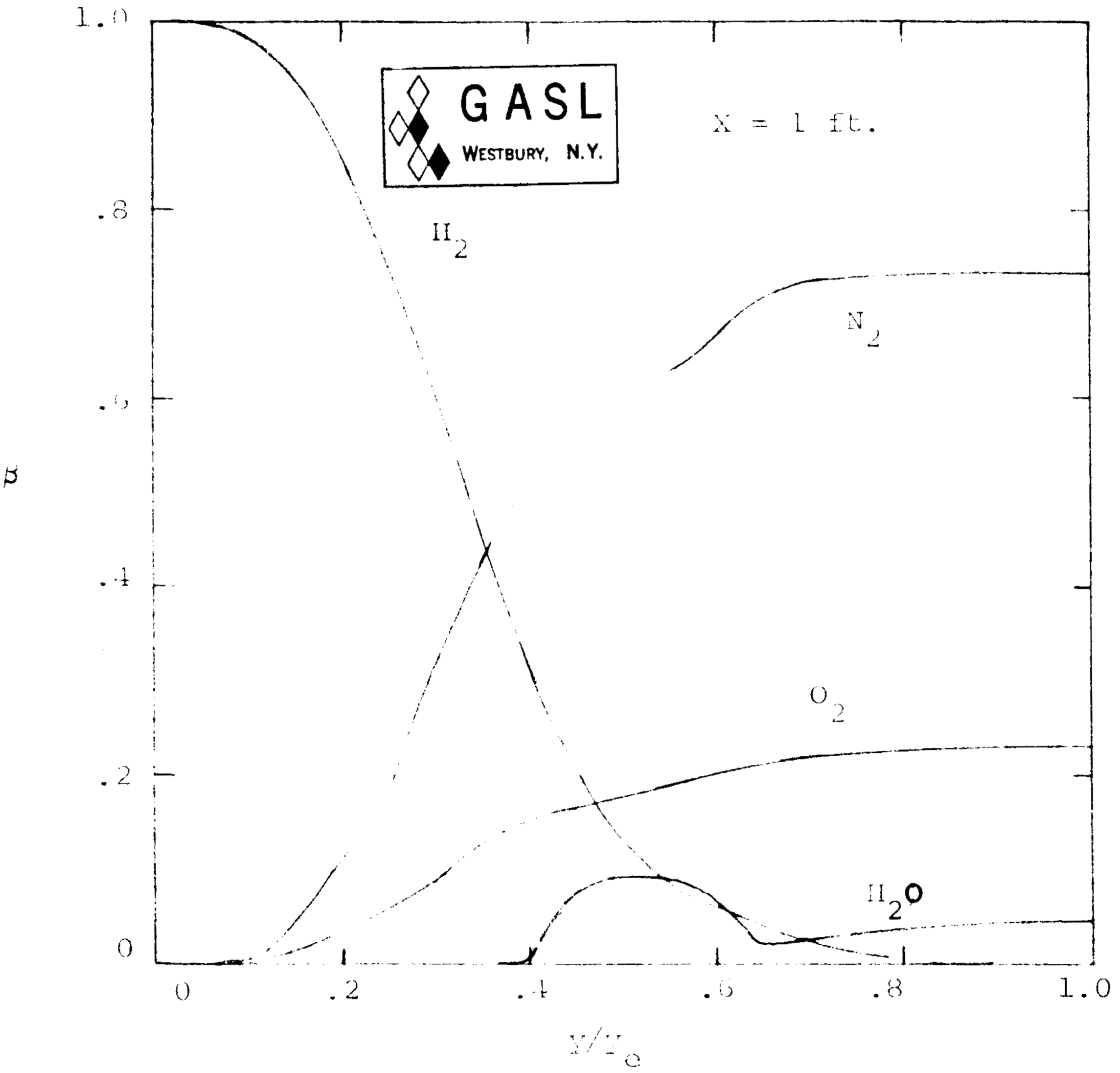


FIGURE 22a - Radial Distributions of the Mixture Mass Fractions

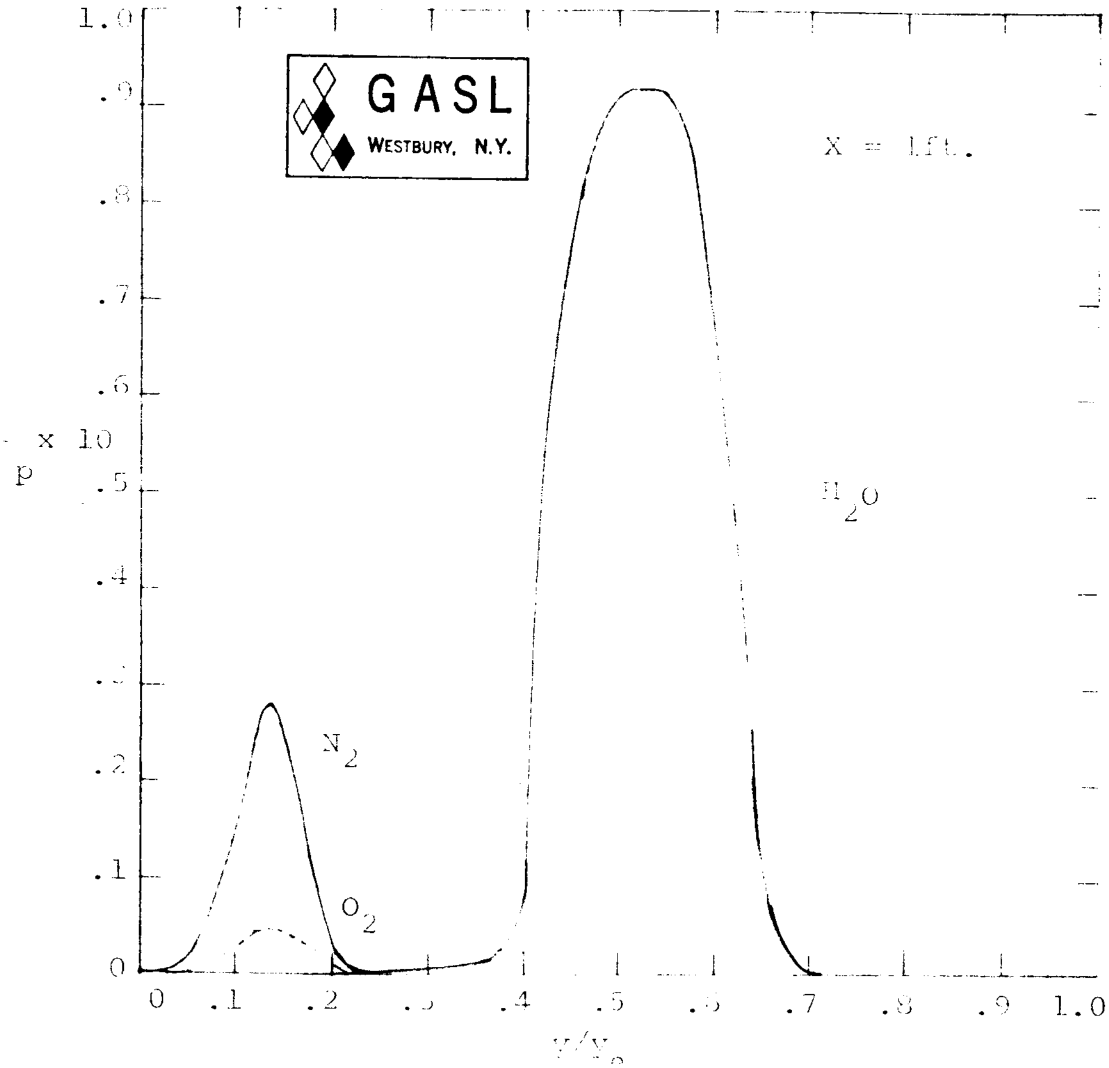


FIGURE 22b- Radial Distribution of the Condensed Phase Mass Fractions

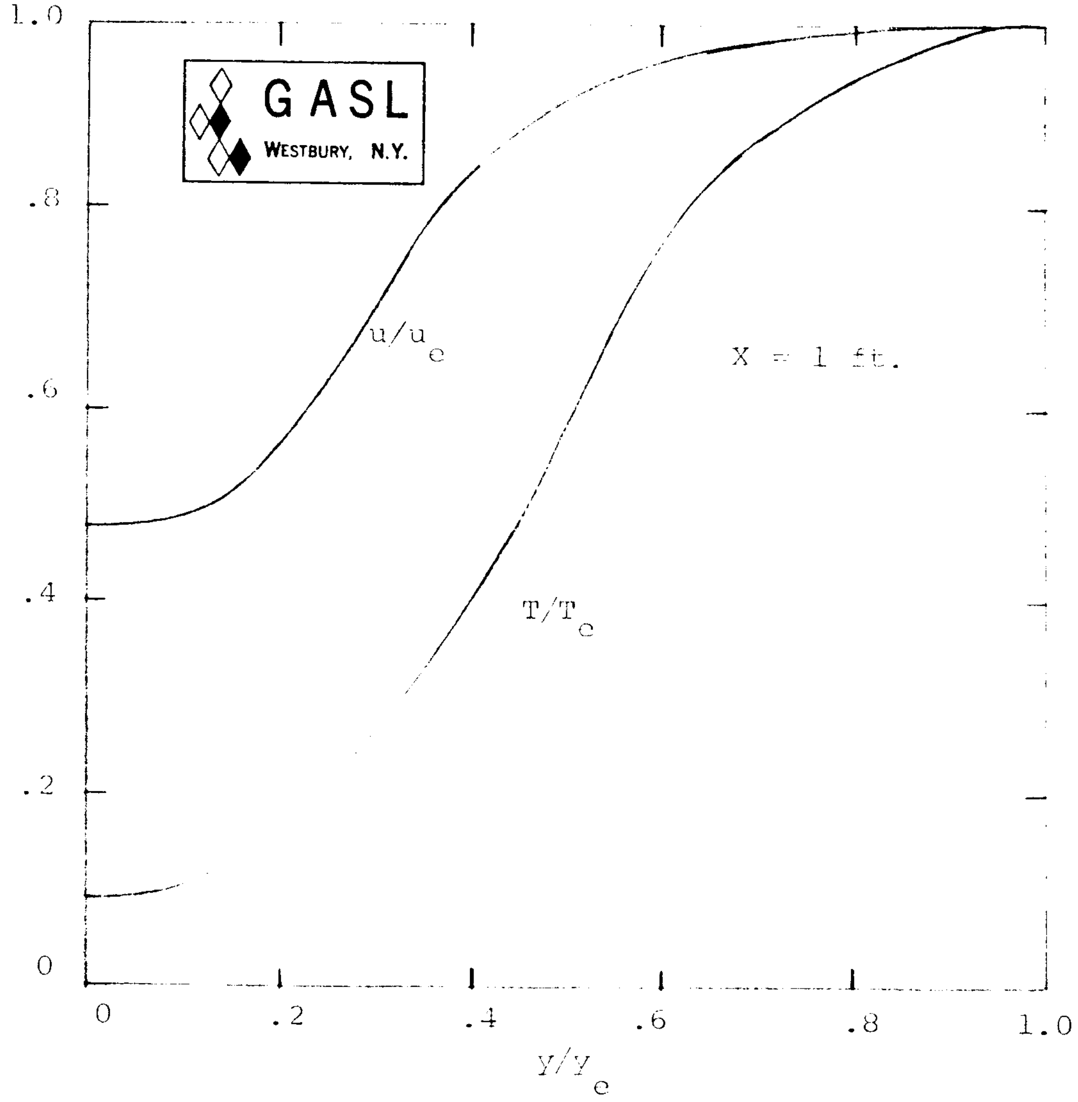


FIGURE 22c-- Radial Distributions of Velocity and Temperature

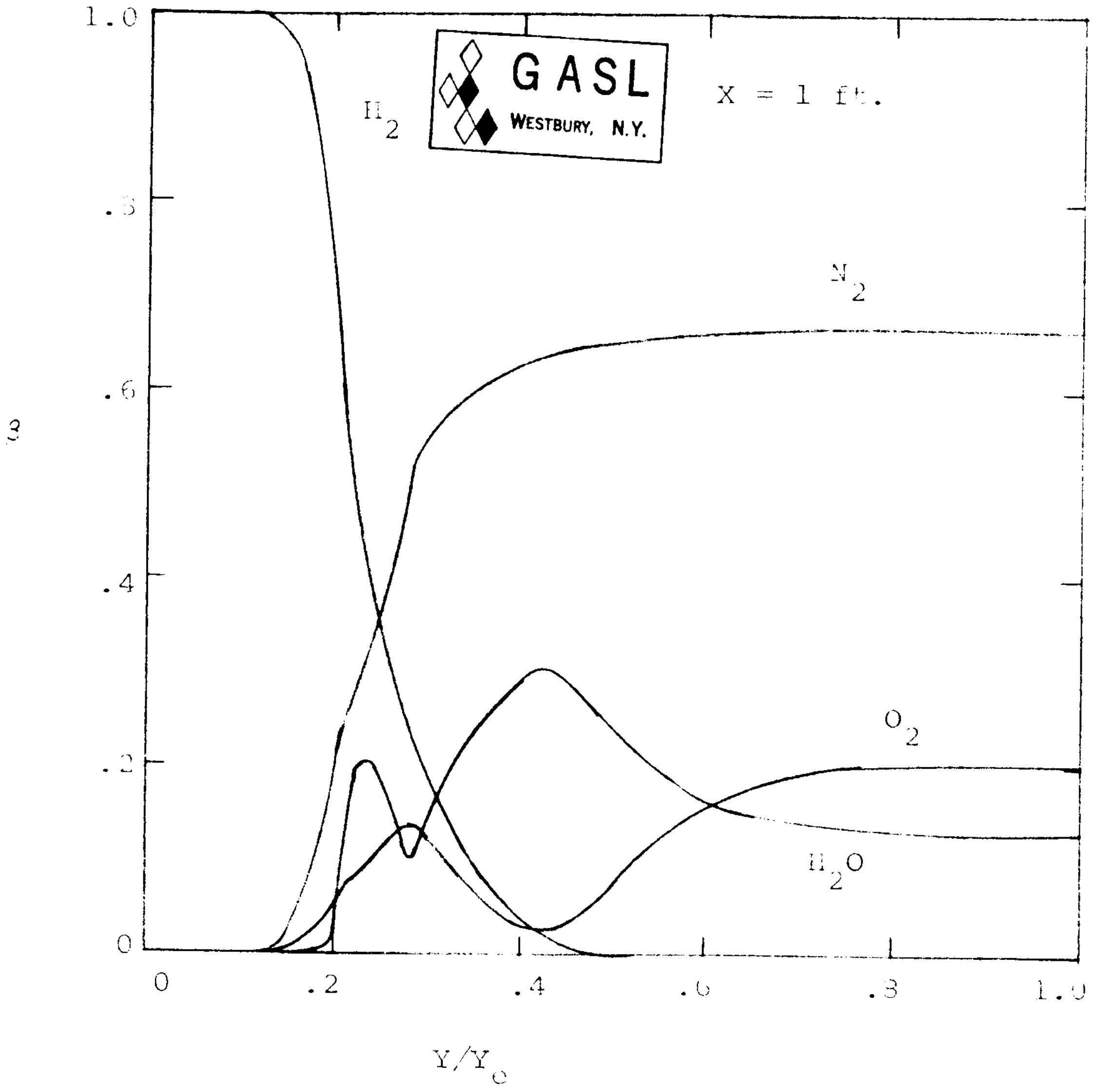


FIGURE 23a - Distributions of the Mass Fractions of H_2, O_2, N_2 and H_2O in the Chemically Reacting Two-Phase Flow

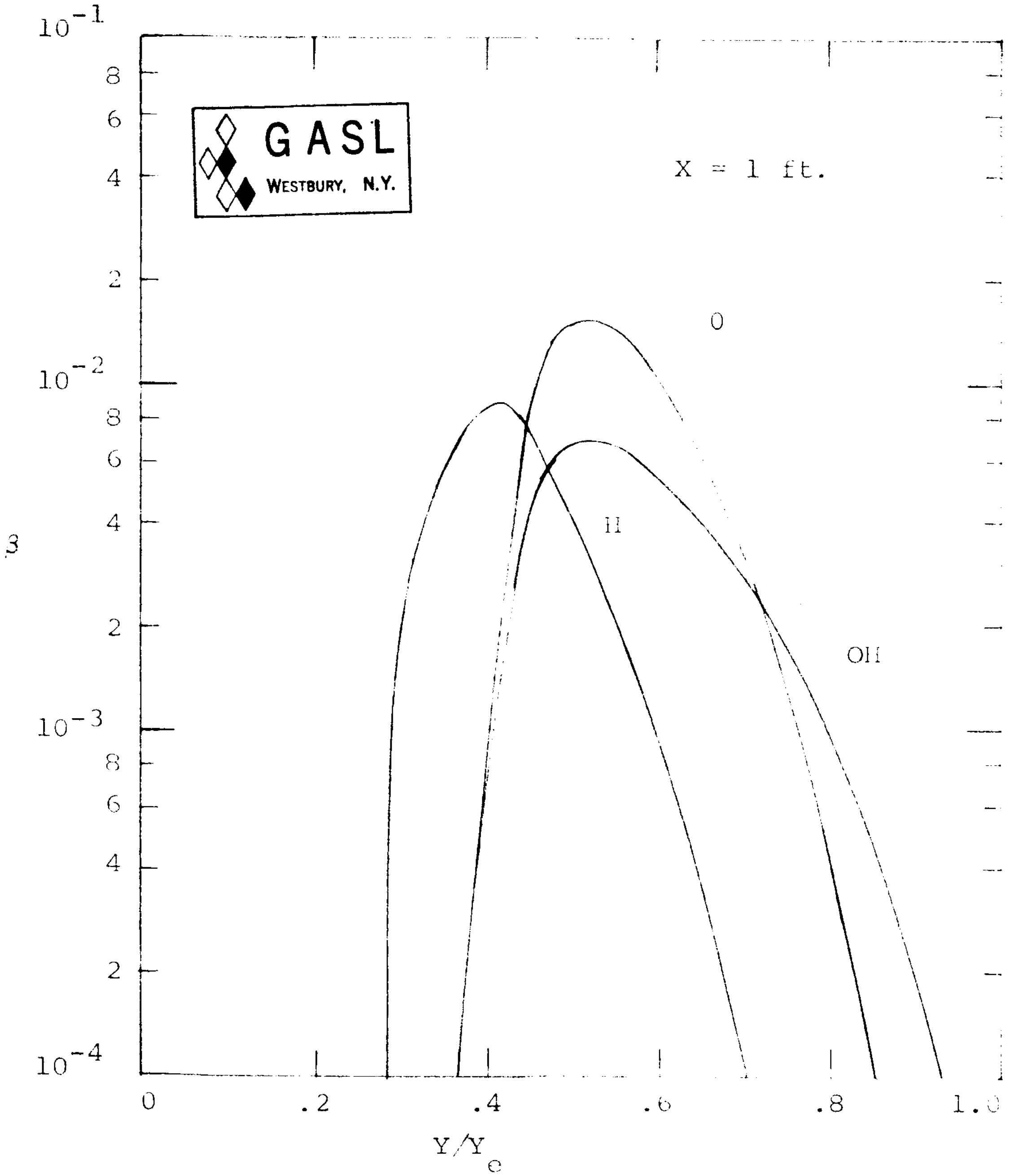


FIGURE 23b - Distributions of Mass Fractions of O,H, and OH in the Chemically Reacting Two-Phase Flow

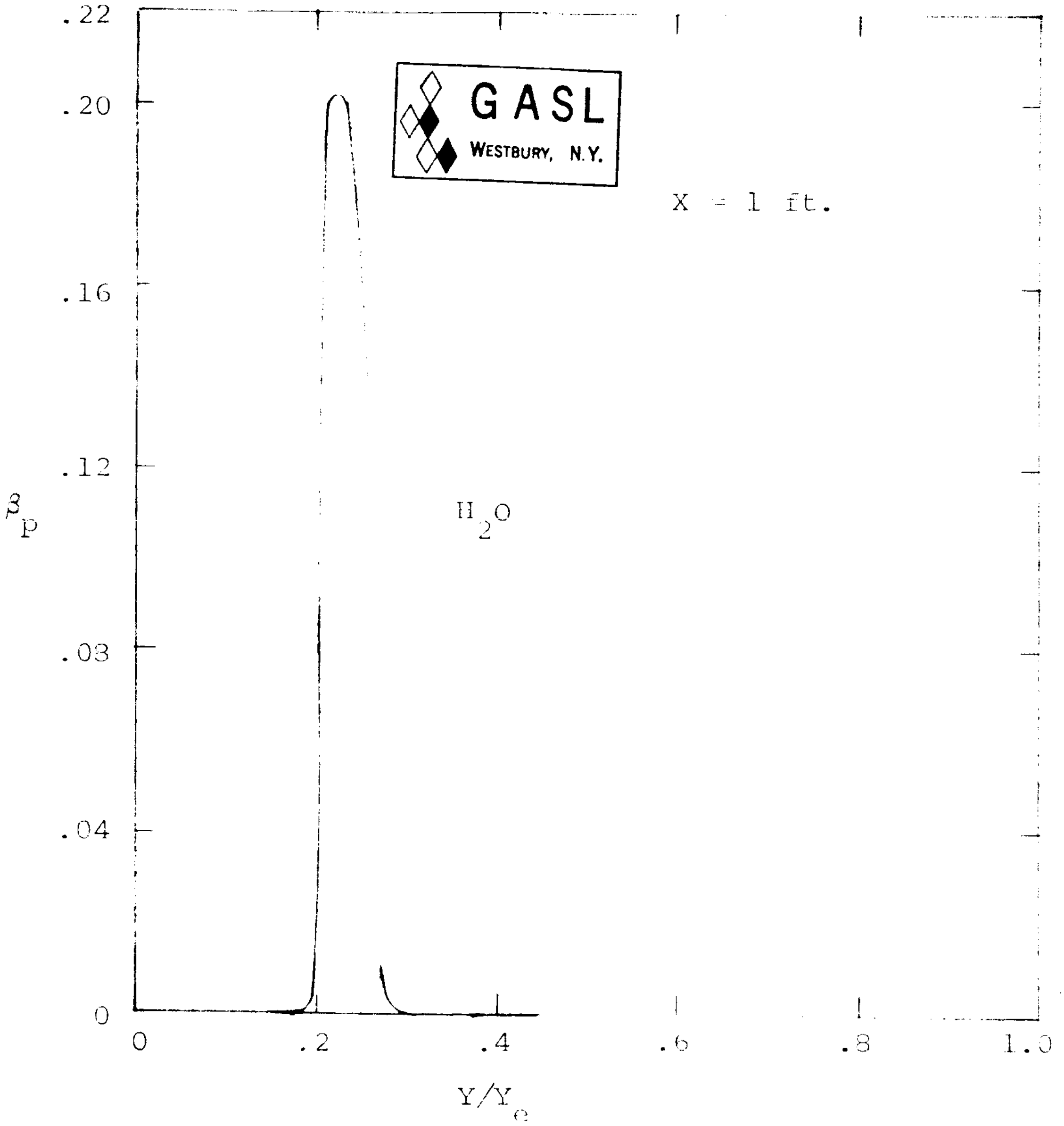


FIGURE 23c - Condensed Phase Mass Fraction Distribution in the Chemically Reacting Two-Phase Flow

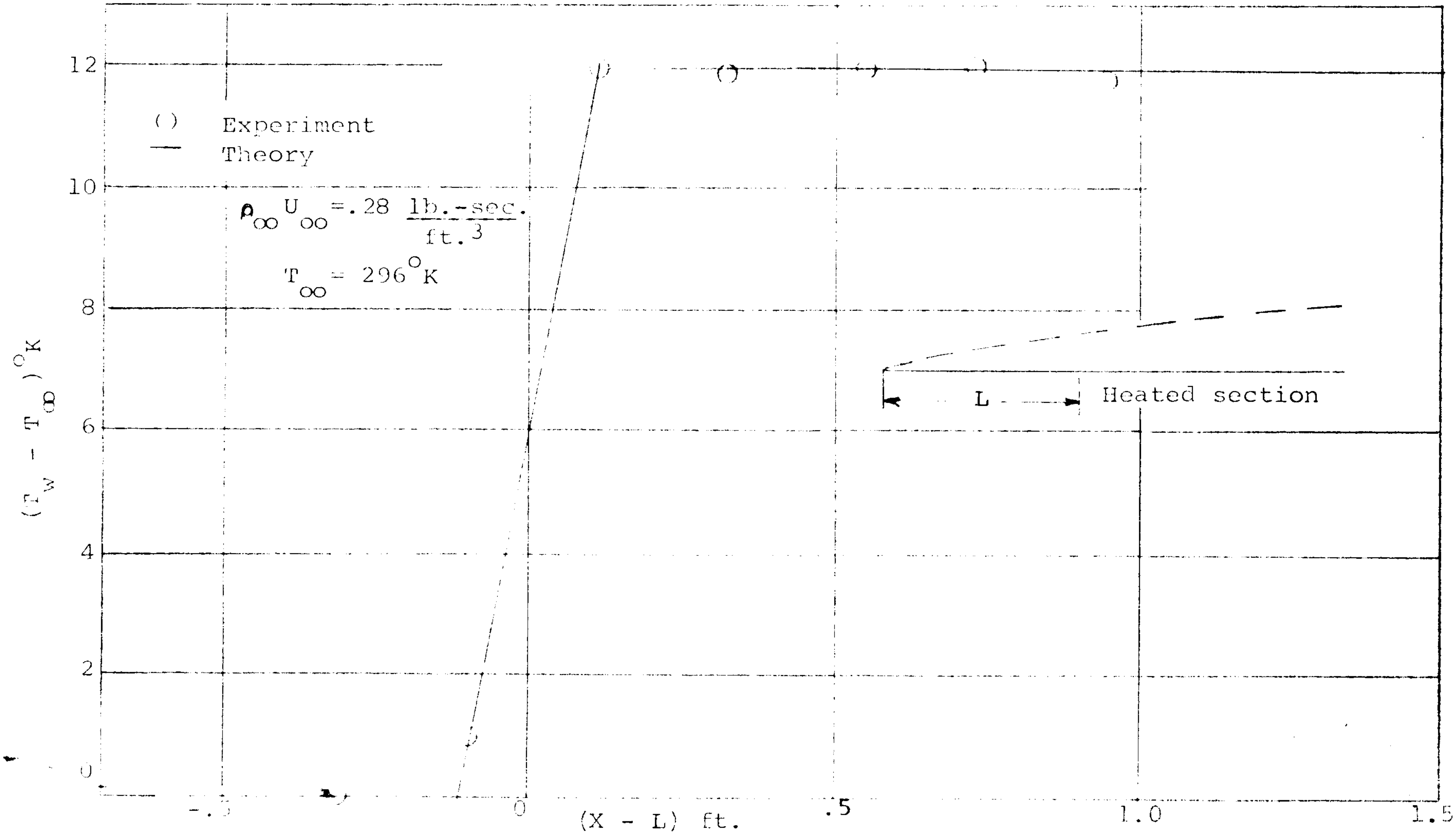


FIGURE 24 Wall Temperature Distribution

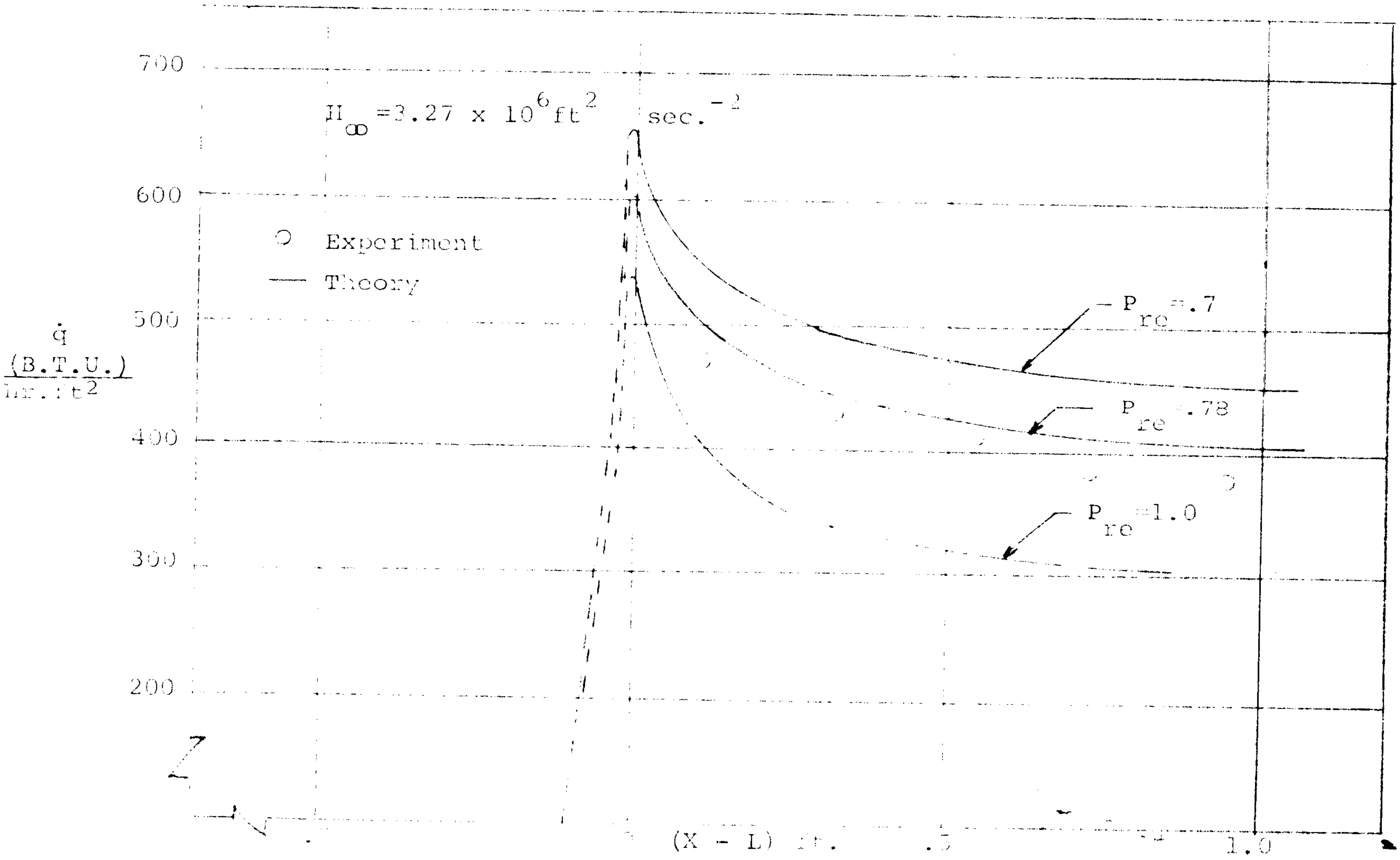


FIGURE 25 Heat Transfer Distribution

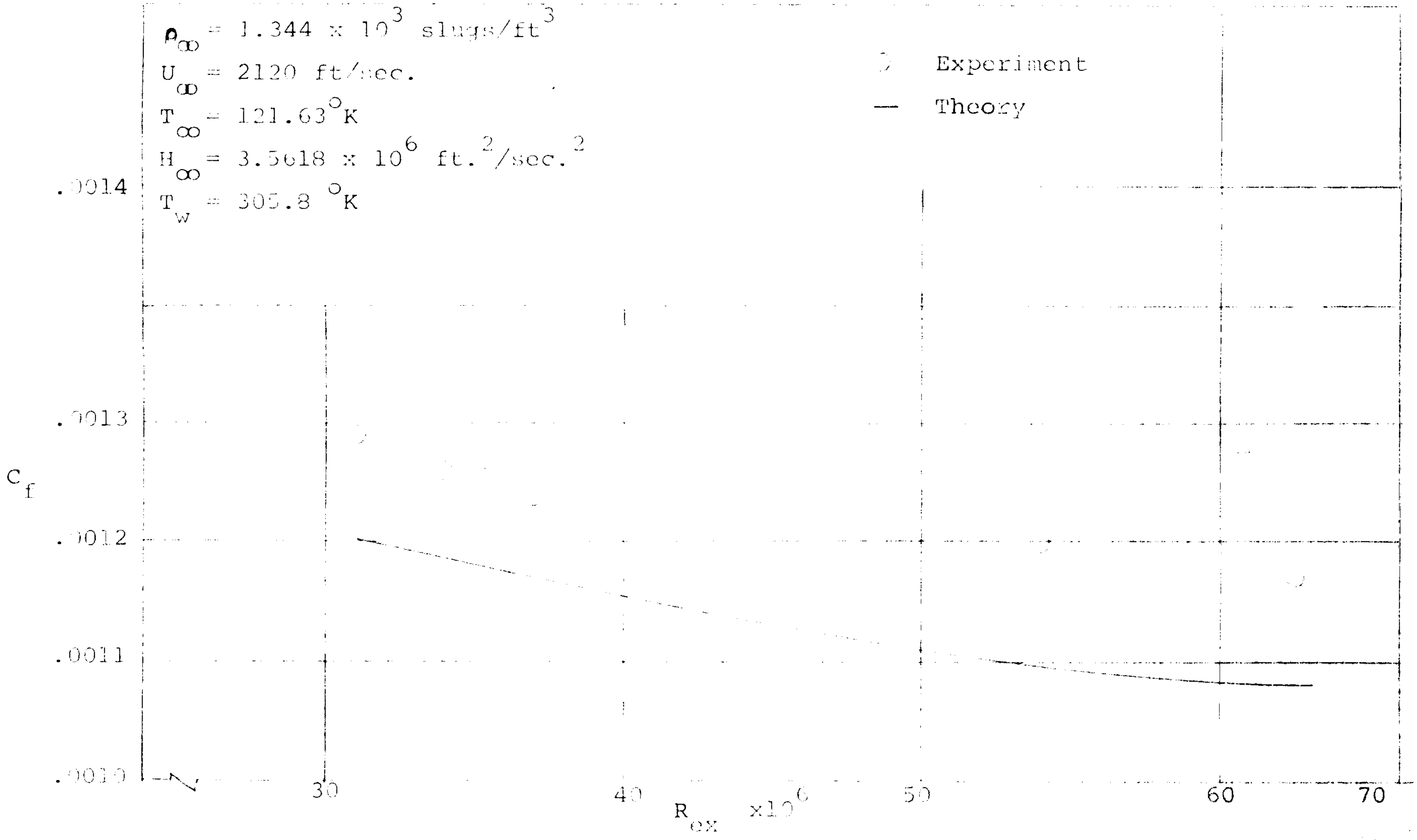


FIGURE 26 Distribution of C_f

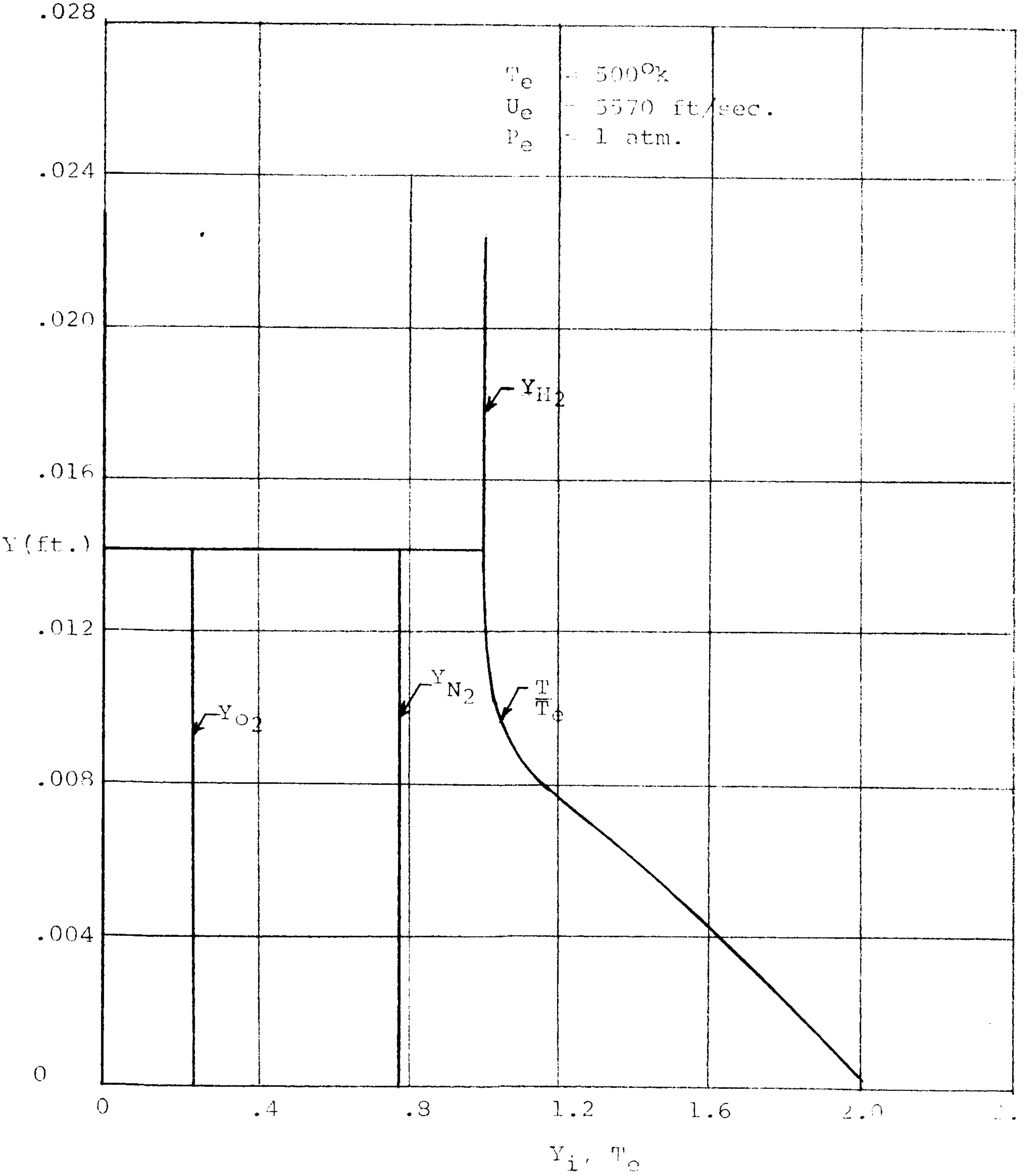


Figure 27 - Initial Distributions of Species and Temperature ratio

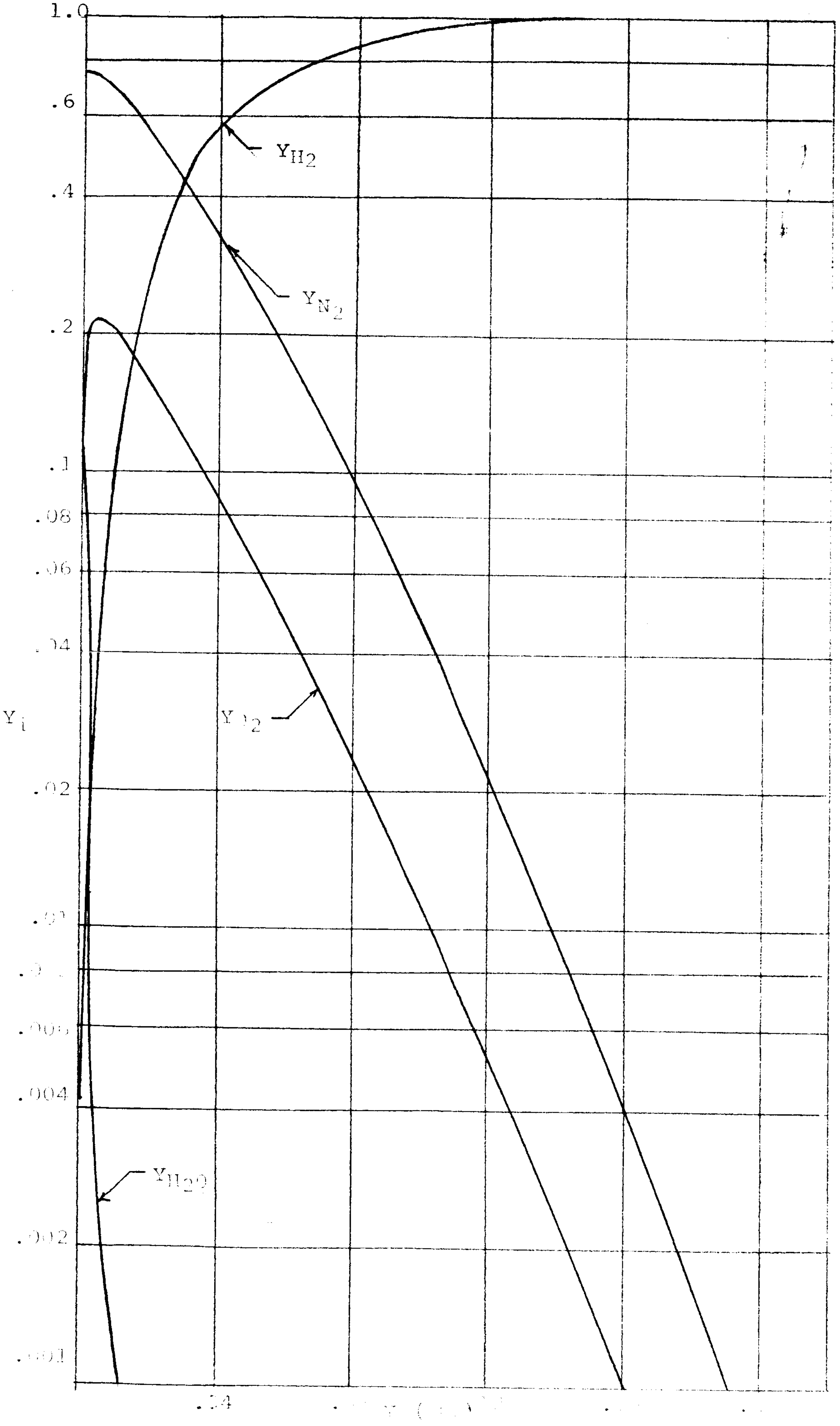


Figure 29 Radial Distribution of [illegible] Mole Fractions, X = .65 ft.

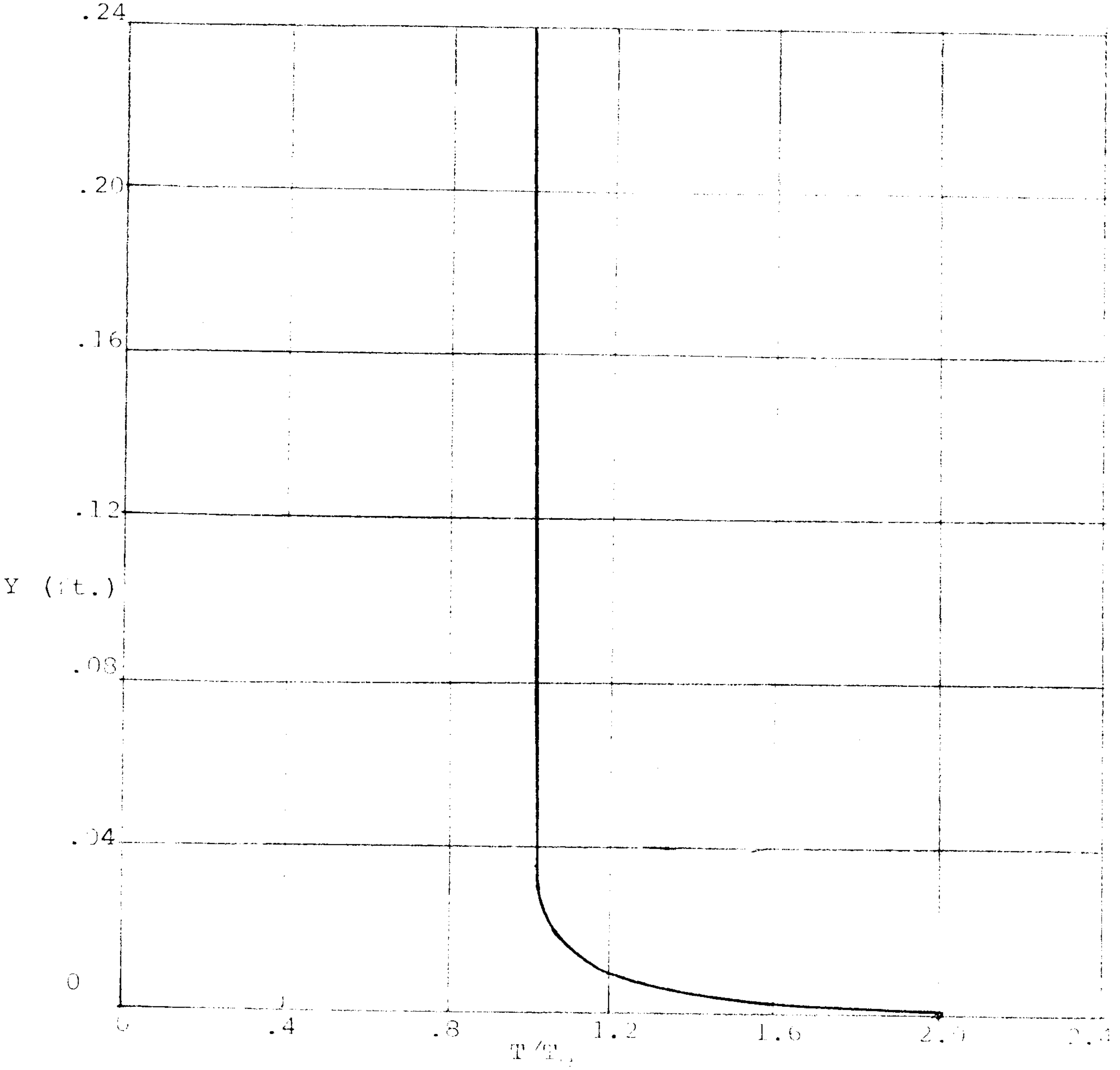


Figure 30 Radial Temperature Distribution, X [illegible]

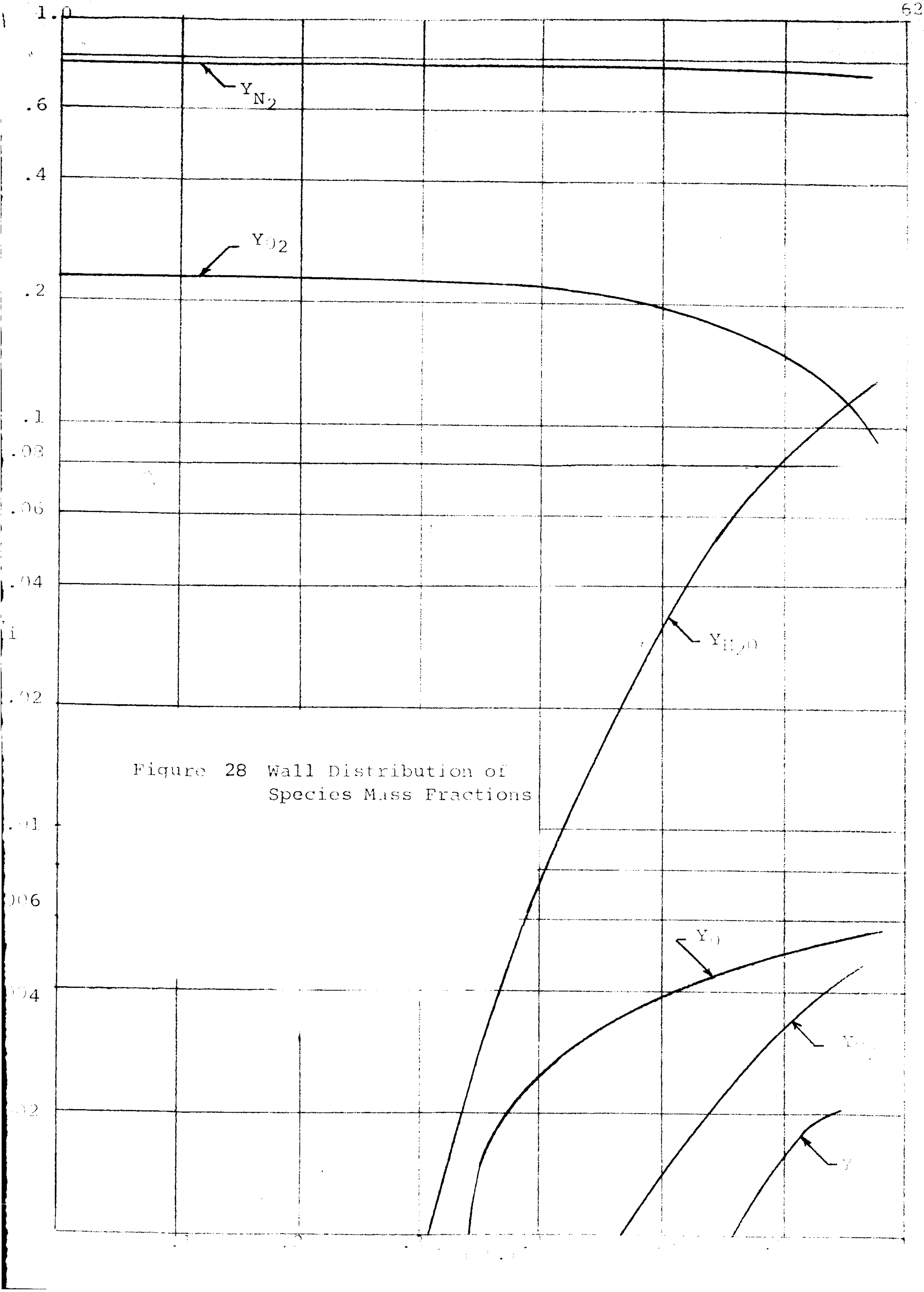


Figure 28 Wall Distribution of Species Mass Fractions