

MIXING OF HOT STARTING JETS

WITH COLD SURROUNDINGS

by

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ABSTRACT

The physical problem considered is that of the hot turbulent starting jet which is formed when hot gases are suddenly ejected through a small nozzle and mix with cold surroundings. The 'pressure-correction' numerical method is employed for solving the two-dimensional, time-dependent Navier-Stokes type of equations which govern the transport of momentum, enthalpy and matter in the mixing process. In this method, velocities and pressure form the aerodynamic dependent variables and the solution is obtained by using a forward-marching technique in time-dimension.

A two-equation turbulence model characterised by the turbulent-kinetic energy and its dissipation rate is employed in the prediction. The model has been tested for its applicability against the experimental data of isothermal, two-dimensional, starting-jet of uniform-property fluid. The rate of chemical reaction is calculated using either a modified version of the 'eddy-break-up' model or an Arrhenius 'global' expression.

Predictions are obtained for two main classes of flows, one in which the hot starting-jet mixes and subsequently ignites the surrounding mixture and the other in which mixing does not result in ignition. In the former case ignition is indicated by a rapid increase in local temperature and pressure and decrease in local fuel concentration to be followed by the hot-gas expansion in the wake of the propagating flame front, while in the latter case no sudden change of the corresponding variables is observed.

The accuracy and validity of these predictions are examined in the light of the available experimental evidence. The good agreements observed between the predicted results and experimental data indicate

not only the correctness of the mathematical representation of the flows but also the capability of the 'pressure-correction' method to predict the present time-dependent problem.

An experimental programme has been included to determine the developments of velocity and temperature at the nozzle exit. A piezo-électric pressure transducer and a set of three thermocouples have been employed in the investigation. The results obtained provide the boundary conditions required in the prediction procedure.

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CHAPTER 1

INTRODUCTION

1.1 Description of the phenomenon and its practical relevance

A starting jet flow under the present investigation occurs when a hot gaseous stream is suddenly released through an orifice of a high-pressure reservoir into cold low-pressure surroundings which may be flowing or stagnant. Immediately after the release the reservoir gases inject into and mix with the ambient gases, setting the latter in motion. If the reservoir pressure is not too high, a sub-sonic starting-jet will be formed as shown in fig. 1.1-1. As the jet penetrates further, it entrains more ambient gases resulting in the increase in temperature of the latter and, at the same time loses heat to the surroundings. If the reservoir capacity is large enough, the mixing process will continue until equilibrium between reservoir and ambient pressures has been reached, then the jet temperature will drop to that of the surroundings.

Fig. 1.1-2 illustrates the expected distribution of axial temperature at different time intervals before the attainment of the equilibrium. Two cases are considered, one in which both the surrounding and the injecting gases are chemically inert and the other in which only one of them consists of the combustible mixtures. For both cases, the continuous injection of hot gases through the opening will result in the increase with time of the temperature at any given point in the flow field. But a decrease in temperature may be observed along the jet-axis away from the opening for the first case as shown in the diagram [case (a)]. If the combustible mixtures are present, the chemical reaction taking place may result in the occurrence of ignition provided that the conditions are favourable,

i.e. the temperature of the emerging jet is not too low and the mixture concentrations of the reactive species are within flammability limits. Ignition is usually followed by a rapid spreading of the flame into the ambient atmosphere causing a sharp rise in temperature as indicated in the diagram for case (b). If ignition does not occur, the estimated temperature distribution will resemble that of case (a). The factors which determine the mixing and the possibility of ignition/non-ignition are the velocities, properties, state and composition of the injecting and surrounding gases and the geometry and size of the orifice.

The starting-jet problem occurs in many engineering processes of practical importance, e.g. the ejection of hot gases from the flange gap of flame traps or flame-proof enclosures, the ignition of fire damp atmosphere by the hot gases coming out of flame-proof enclosures or by hot jets of exhaust products of dynamite explosives used for blasting, the bursting of the diaphragm of a safety valve caused by an excess pressure of the reservoir fluid, the sudden opening of the discharge valve of a pressure vessel and the injection of fuel into a combustion chamber of engines. Thus in the design of many engineering equipments, the understanding of starting-jet flow is of immense value particularly in safety considerations. The designers would want to know not only qualitatively but also quantitatively the influence of various parameters and the way in which they affect the flow characteristics. A full-scale experimental investigation, though yielding the required information, is usually expensive and time-consuming. An alternative is to develop a calculation procedure which is capable of predicting the phenomenon correctly and economically. To achieve such an objective, the mathematical model must be constructed to represent as closely as possible to the flow and the mathematical technique employed to obtain solution must be efficient. This

procedure, once it has been verified, can be used with confidence and considerable savings both in time and expense to improve the design of various related engineering equipment.

The prime objective of the present thesis is to develop such a calculation procedure for the study of the mixing-process between the hot, turbulent, round-sectioned gaseous starting-jet and cold surroundings. In the investigation, the factors affecting the mixing are taken to be the velocity, temperature and composition of the jet and those of the surroundings. The validity of the procedure will be shown to be confirmed by the favourable comparison of predictions with existing experimental data. As the physical situation considered here resembles that of the ignition of fire-damp atmosphere by hot jets mentioned earlier, the present results can directly be used in the study of prevention of explosion hazards in mines. It is in fact this particular practical relevance that prompts the Safety in Mines Research and Establishment (U.K.) to provide financial support for the project.

1.2 Previous work

1.2.1 Theoretical investigations

Despite its practical importance, the starting-jet phenomenon has not been much investigated in comparison with that of the steady-jet. This is mainly due to the lack of (i) a computing tool powerful and efficient enough to deal with the Navier-Stokes governing equations which are three-dimensional in nature and (ii) a knowledge of the physics of

of the unsteady turbulent mixing process involved. To overcome the first hindrance, the assumptions of boundary-layer and incompressible flow are usually introduced in most of the early studies to allow the governing equations to be simplified into the form which can be solved by analytical or simple numerical methods. The second difficulty is often by-passed by either channelling the investigation to that of the laminar case or using a simple mathematical model of the steady-flow to characterise the mixing.

Bhuta and Page (1961) obtained an analytical solution for incompressible, laminar (or turbulent), two-dimensional unsteady jet by linearising the Prandtl boundary-layer equation using the method of perturbations. The method, though comparatively simple, is only applicable to the case where the velocity along the main flow direction is very much larger than that normal to the main flow. Kent (1973) presented a numerical solution based on the integral method for the same problem. This method assumes the similarity in the nature of the flow and ignores the effect of pressure gradient in the flow field. The similarity assumption was also employed by Ma and Ong (1971) and by Wirz (1973). Wirz investigated the compressible, two-dimensional, unsteady jet mixing but his study was again restricted to that of boundary layer flows. In his method, the similarity variables are introduced in the transformation to eliminate the density from basic equations and as a consequence the number of governing equations to be solved has been reduced.

The solution of the fully two-dimensional unsteady equations was firstly obtained by Payne (1958) for the starting-jet at a low Reynolds number. He solved the Helmholtz's vorticity and continuity equations simultaneously using a step-by-step time-interval method with the forward and central finite-difference formulation being applied respectively in the

calculations of the time and spatial derivatives. By replacing the central finite-difference with the upwind difference, Ma and Ong (1971) were able to extend the calculation to cover high Reynolds number cases. Their approach is however different from the one employed by Payne. The method involves the use of similarity variables to transform the three-dimensional governing equations into two-dimensional ones and the latter are solved by a Gauss-Seidal iterative procedure. Although the predictions agree well with experimental findings reported in the same paper, the 'similarity' method possesses an important limitation. It is limited to problems possessing similar-solutions which, for starting-jet flow, are achieved only at large axial distance downstream of the nozzle. For the flow close to the nozzle the method cannot provide satisfactory solutions. To overcome this shortcoming, Hengrussamee et al (1973) developed Payne's time-interval method in which flow patterns may be obtained at each successive interval of time. This method removes the limitations embodied in the previous two techniques except the incapability to deal with flows of variable-density fluids.

All investigations reviewed so far are mainly concerned with aerodynamic behaviour of the isothermal starting-jet. The attempts to study starting flows with temperature gradients and chemical reactions have been minimal. The only theoretical treatment of this particular problem was carried out by Phillips (1971) in his investigation of the suppression of explosion by narrow gaps. He assumed that the ignition of combustible surrounding mixtures occurs in a spherical vortex at the head of the turbulent starting-jet emerging from the gap at some distance downstream. Consequently a one-dimensional energy balance was performed for a small gas pocket inside the vortex and the resulting ordinary differential equation was solved to give the maximum safety gap. This

one-dimensional approach is however inadequate for the detailed study of the phenomenon which is two-dimensional and time-dependent. Thus a new prediction procedure with two-dimensional capability is required.

Numerical solutions of the Navier-Stokes equations have proliferated in recent years due to the improvement in the capacity and speed of the electronic computer. The range of these solutions has expanded rapidly and several techniques have been developed to high degrees of sophistication. Some of these techniques relevant to the present study are reviewed. Thommen (1966) proposed a numerical integration method based on the 'two-step Lax-Wendroff' stable forward-difference scheme for the solution of two-dimensional unsteady compressible flows of inviscid fluid. The procedure employs two-step time-intervals the first of which may be referred to as the intermediate step and the second is the step where solution is sought. The second-step velocity is obtained through the use of finite-difference forms of continuity and momentum equations after the intermediate velocity fields have been computed based on Taylor expansion. However this method proves to be unsuitable because of its uneconomical nature which results from the use of Taylor expansion and two-step intervals and also its restricted application to inviscid flows only. The solutions for viscous fluid of the Navier-Stokes equations were later obtained by Chorin (1968) and Amsden and Harlow (1970). Both used the single step time-interval finite-difference methods with velocity and pressure as dependent variables. The two methods are very similar in their basic ideas; the velocity fields are first estimated with the use of momentum equations and the continuity equation is subsequently employed to correct them. While Chorin ignored the pressure gradient effect in his estimation of velocities, Amsden and Harlow solved the full momentum equations using the guessed pressure fields. To correct

these velocities, Chorin solved a form of Poisson's equation for pressure which may be derived from the continuity equation, while Amsden and Harlow introduced a potential function into the computations. Patankar and Spalding (1972) adopted the technique based on such ideas to predict three-dimensional boundary-layer confined flows of uniform-property fluid. The use of pressure as a main dependent variable has made it convenient for the application of these velocity-pressure methods for the unsteady, two-dimensional, non-isothermal, non-uniform density jet flows. Moreover the readily available knowledge of pressure distributions obtained will be very valuable in providing understanding of the investigated phenomenon.

The survey of the theoretical study of the starting-jet will not be completed without the discussions of further mathematical models which portray the physics of the flow. Two models are presented here, one which describes the turbulent motion and the other which specifies the chemical reaction.

Turbulence model. In the attempts to construct a mathematical model of turbulence, the following two main approaches are usually considered. The first was proposed by Boussinesq (1877) who replaced the stress terms appearing in the momentum equations with new terms containing the products of effective viscosity and local velocity gradients. To complete the construction of the model, the effective viscosity must subsequently be prescribed or related to other calculated dependent variables. The second approach is based upon the way in which the system of governing equations prescribing turbulent motions is closed. For example, a further set of equations representing the conservation of these stresses may be derived, and these equations together with the time-averaged momentum and continuity equations will form the closure.

Categorised under the first approach are the two-well known models

which have been applied successfully to evaluate the effective viscosity; they are Schlichting's uniform viscosity model (1968) and the Prandtl's mixing length hypothesis (1925). As these models can only be employed for boundary-layer types of flows, their success is rather limited. Attempts to obtain more general and accurate representation of turbulent flows lead to the development of more sophisticated models in which the effective viscosity is assumed to be a function of two turbulent quantities. Kolmogorov (1942) and Prandtl (1945) both proposed a differential equation for turbulent kinetic energy and an algebraic expression for a length scale in their model. Rotta (1951) employed the same variables but replaced the prescription of length scale with another differential equation expressing its conservation. Launder et al (1972) adopted a similar two-equation turbulence model approach with the dissipation rate of turbulent kinetic energy as the second turbulent variable in place of the length scale. Not only can these models predict more accurately the boundary layer flows, they can also be applied to obtain solutions for flows with recirculation [Le Feuvre (1973)].

The second approach, because of its mathematical complexity and also excessive computing-time requirements, has been employed only in dealing with the simplest of the practical situations. Hanjalic and Launder [Launder et al (1972)] have applied this approach to predict a limited number of boundary layer flows with satisfactory results. For more complex problems, the model has not been well tested due to the difficulty in performing accurate measurement of the triple-correlation quantities required in the determination of constants used in the model.

No one has so far postulated any model for unsteady turbulent flows. Because of the lack of such information, Ma and Ong (1971) made use of Schlichting's uniform effective viscosity model. Although the predictions

were found to be satisfactory, the model is not realistic and is incapable of predicting flows of variable-property fluid. The two-equation model, on the other hand, can be tailored to take into account the variation of effective viscosity with time. The most developed model of this kind is based upon the use of turbulent kinetic energy and its dissipation rate as turbulent variables [Launder et al (1972)]. While this model has been applied extensively to various steady-state problems, its application to unsteady phenomenon is still very novel. The present work makes a contribution in this line by applying the model to the prediction of two-dimensional, unsteady, non-isothermal starting-jet flows.

Chemical reaction. In combustion processes, fuel and oxygen combines through many complex steps forming many intermediate radicals before the final stage is reached. The conclusions drawn from the investigations of multi-step methane-oxidation mechanism by Asaba et al (1963) and Seery and Bowman (1970) indicate that the types of radicals formed and the number of chain reactions involved depend not only on the experimental set-up but also on the prevailing ambient conditions. Such uncertainty coupled with the large computer-time which would be required in the numerical study of the present problem have made this approach unattractive. Thus a global reaction rate model which assumes that fuel and oxygen combine at a finite rate in a single-step to form combustion products is usually employed in preference. The use of this approach raises the question of how the rates of fuel and oxygen consumptions are to be determined. The most common and straightforward way is to assume chemical kinetic control prescribed by the global Arrhenius expression. Because of its simplicity and also the lack of other suitable alternatives, this reaction model has been employed most frequently in the

prediction of combustion phenomena [Goh and Ma (1970 and 1972), Phillips (1971)]. Spalding (1970) proposed the 'eddy break-up' model in which the local state of turbulence as well as chemical kinetics are allowed to exert their influence on reaction. In this model, the effective reaction rate is taken to be the lower of the following two rates, the rate of dissipation of mass-fraction fluctuations and the rate given by the Arrhenius expression. Stephenson (1972), Mason (1973) and Runchal (1973) have successfully applied the model to obtain predictions for turbulent reacting flows. Although the model appears to be more realistic than that of Arrhenius, it is still in its exploratory stage and needs further investigations before its superiority can be acclaimed, particularly for the pre-mixed scheme under the present investigation.

1.2.2 Experimental investigations

Earlier experimental work on starting-jets were mostly confined to the qualitative study of the flow patterns resulting from the mixing of isothermal homogeneous fluids. Rizk (1955) carried out a flow visualization test for the development of axi-symmetric starting water jet with particular reference to the scavenging process in two-stroke engines. Meyer (1961) used smoke-tracers to follow the mixing of low-velocity air jet with stagnant surroundings. The first quantitative detailed study was carried out by Ma and Ong (1971) in their attempt to verify their predictions of the two-dimensional, air into air, turbulent, starting jet. Traversing hot-wire probes were used to measure the development of streamwise velocity at various stations downstream of the nozzle outlet.

The more practically orientated investigations on starting-jet flows involving non-uniform fields of temperature and concentrations were carried out by Phillips (1971) and Wolfhard and Bruszak (1959). Both experiments were directed towards obtaining the maximum safe-gap size which prevents the transmission of flames from the inside of an enclosure into inflammable surroundings. Phillips took Schlieren photographs of the development of hot, sub-sonic jet emerging from a small nozzle mounted on an explosion cylinder which was also fitted with large pressure release vents. Ignition or non-ignition phenomenon resulting from the mixing of this jet with surroundings was obtained by suitable adjustment of the composition of the mixing media. Wolfhard and Bruszak carried out a similar investigation but they employed a sealed explosion-cylinder placed in an inflammable atmosphere which is enclosed inside a large duct.

1.3 The present contribution

The main contributions of the present thesis may be summarized as follows:

1. A calculation procedure capable of predicting accurately the mixing of hot, turbulent, round-sectioned, starting-jets with either inflammable or chemically inert surroundings has been developed. The investigation involves the formulation of mathematical models to represent the physical situation and the use of a velocity-pressure numerical approach to solve the resulting unsteady two-dimensional governing equations. The transient distribution of pressure which is instrumental to the understanding

of the phenomenon and was hitherto impossible to obtain, is presented.

Preliminary tests on the applicability and accuracy of the procedure have been systematically carried out against known analytical or numerical solutions of the related but less complicated problems. Encouraging results enable the procedure to be adopted to predict the present phenomenon.

2. The procedure has been employed to determine the appropriate physical input regarding turbulent flows for unsteady-jet problem. Existing experimental data obtained by Ma and Ong (1971) for isothermal air-air injection are used in the investigation.

3. An experimental programme has been carried out to follow the developments of temperature and velocity of the hot jet injecting into air at the nozzle exit. The data are fed into the calculation procedure as the boundary conditions.

4. The theoretical predictions have been compared with Phillips' experimental data (1971) for both non-ignition and ignition cases. The good agreements between the two results demonstrate the validity of the calculation procedure.

1.4 Outline of thesis

The main body of the thesis consists of six chapters the first of which has just been described.

The second chapter starts with the detailed description of the physical problem under investigation. This is followed by the mathematical statement for such a problem which includes the governing equations, the turbulence model, the transport and thermodynamic properties of mixing fluids, the chemical reaction models and the associated boundary conditions.

The chapter ends with the presentation of the final set of the governing equations.

In the third chapter, the numerical method used to solve the equations is described. The chapter commences with the general discussion on the logic and basic themes of the velocity-pressure approach. The finite-difference equations representing the governing equations and their solution procedure are then reported. Special treatments to incorporate the non-uniform density effect and to procure convergence and stability of the procedure are presented. The numerical procedure is then tested before it is applied to obtain predictions of the present problem. In the final section, the predicted results are presented and discussed.

Chapter 4 is concerned with the experimental investigation to obtain the developments of temperature and velocity of the jet at the nozzle outlet. The chapter describes the general arrangement of the apparatus, the instrumentation and the measuring procedure. The experimental results are then discussed, analysed and later put into the form ready to be used as boundary conditions for the predictions. Finally Phillips' experimental data are prepared for the comparisons to be made in the next chapter.

In chapter 5, the predicted and experimental results for the non-ignition cases are compared and discussed. The comparisons are then extended to cover the ignition-cases. The following section includes a summary of principal results and the discussions on the capabilities of the prediction procedure, the turbulence and chemical reaction models. The thesis ends with recommendations for future work and the main conclusions of the present study.

After the main body, the nomenclature, list of references, the figures and the photographic plates are presented consecutively. This is

followed by the four appendices, the first of which describes the derivation of wall functions employed to characterise the flow in the near-wall region. The second appendix illustrates the transformation of governing partial differential equations into finite-difference forms. In the third appendix, the derivation of the relationships employed in the determination of the velocity and temperature developments are presented. The last appendix consists of tables of experimental results.

CHAPTER 2

MATHEMATICAL STATEMENT

2.1 Introduction

The problem under the present investigation is depicted in fig. 2.1.1. A combustible mixture of methane, oxygen and nitrogen inside the vertical explosion cylinder which is fitted with two pressure release vents at its base, is spark-ignited. The resulting hot gases escape through a small nozzle at the top of the vessel and mix with the cold stagnant surroundings. A sub-sonic, round-sectioned, turbulent starting-jet is thus formed. Whether this jet can ignite the surroundings or not will depend upon the velocity, temperature, composition of the jet and those of the surroundings and also the diameter of the nozzle.

The mixing process of a hot starting jet with cold surroundings is governed by the time-dependent partial differential equations which express the conservation of mass, momentum, enthalpy and species. The assumption of the flow as being axisymmetrical enables these equations to be reduced to a time-dependent two-dimensional set which can be solved by a numerical technique to be reported in details in Chapter 3. However before this can be done, the turbulent motion in the flow and the chemical reaction taking place between reactive species there must firstly be prescribed. In the present study, the turbulent effect is assumed to be adequately represented by two differential equations of the Navier-Stokes type governing the conservation of two turbulent quantities and the chemical reaction to obey an algebraic relationship linking the reaction rate to other calculated variables and fluid properties in the analysis.

The chapter will commence with the descriptions of fundamental equations and other important auxiliary information. These will be followed by the discussions of turbulence models, the evaluation of transport

and thermodynamic properties, the characteristics of boundaries and the modelling of chemical reaction. The boundary and initial conditions required in the solution of these governing equations will then be given. In the closure, the final set of equations which have been obtained uniquely for the present investigation is presented.

2.2. Governing equations

The time-dependent set of equations, for an unsteady axisymmetrical, non-uniform density, turbulent jet mixing coupled with chemical reactions may be written with reference to the cylindrical co-ordinates (z, r, t) as:

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho W)}{\partial z} + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V) = 0 \quad (2.2.1)$$

Momentum equations:

$$\frac{\partial}{\partial t}(\rho W) + \frac{\partial}{\partial z}(\rho W^2) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V W) = \frac{\partial \tau_{1,1}}{\partial z} + \frac{1}{r} \frac{\partial}{\partial r}(r \tau_{1,2}) - \frac{\partial P}{\partial z} \quad (2.2.2)$$

$$\frac{\partial}{\partial t}(\rho V) + \frac{\partial}{\partial z}(\rho W V) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V^2) = \frac{\partial \tau_{2,1}}{\partial z} + \frac{1}{r} \frac{\partial}{\partial r}(r \tau_{2,2}) - \frac{\tau_{3,3}}{r} - \frac{\partial P}{\partial r} \quad (2.2.3)$$

Equation for conservation of total stagnation enthalpy:

$$\begin{aligned} \frac{\partial}{\partial t}(\rho H) + \frac{\partial}{\partial z}(\rho W H) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V H) &= \frac{\partial}{\partial z} \left(r \int_H \frac{\partial H}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \int_H \frac{\partial H}{\partial r} \right) + \frac{\partial P}{\partial t} \\ &+ \frac{\partial}{\partial z} \left[(\mu_t + \mu) \left(1 - \frac{1}{\delta_H} \right) \frac{\partial}{\partial z} \left(\frac{W^2 + V^2}{2} \right) \right] \end{aligned}$$

$$\begin{aligned}
 & + \left(\frac{1}{\delta_k} - \frac{1}{\delta_H} \right) \frac{\partial k}{\partial z} + \sum_j \left(\frac{1}{\delta_j} - \frac{1}{\delta_H} \right) h_j \frac{\partial m_j}{\partial z} \Big] \\
 & + \frac{1}{r} \frac{\partial}{\partial r} \left[r (\mu_t + \mu) \left(1 - \frac{1}{\delta_H} \right) \frac{\partial}{\partial r} \left(\frac{W^2 + V^2}{2} \right) \right. \\
 & \left. + r \left(\frac{1}{\delta_k} - \frac{1}{\delta_H} \right) \frac{\partial k}{\partial r} + \sum_j r \left(\frac{1}{\delta_j} - \frac{1}{\delta_H} \right) h_j \frac{\partial m_j}{\partial r} \Big] \\
 & \qquad \qquad \qquad (2.2.4)
 \end{aligned}$$

Equation for conservation of species j:

$$\begin{aligned}
 \frac{\partial}{\partial t} (\rho m_j) + \frac{\partial}{\partial z} (\rho W m_j) + \frac{1}{r} \frac{\partial}{\partial r} (\rho r V m_j) &= \frac{\partial}{\partial z} \left(\tau_j \frac{\partial m_j}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \tau_j \frac{\partial m_j}{\partial r} \right) + \dot{m}_j''' \\
 & \qquad \qquad \qquad (2.2.5)
 \end{aligned}$$

The symbols in the above equations have the following meanings:

- (i) W and V are the mean velocity components in longitudinal (z) and radial (r) direction (z being measured from the nozzle exit and r from the axis of symmetry).
- (ii) ρ , P and t stand for density, pressure and time respectively.
- (iii) τ is the stress term. The first subscript of τ indicates its direction and the second the direction normal to the plane on which it acts. For example, $\tau_{3,3}$ is the normal stress acting in direction 3 (circumferential) on the plane 12(zr) and has its normal parallel to direction 3.
- (iv) H stands for the total stagnation enthalpy which is defined as:

$$H = C_p T + m_f H_f + \frac{1}{2} (W^2 + V^2) + k \qquad (2.2.6)$$

where C_p is the specific heat at constant pressure of the mixture, T the local temperature, m_f the mass fraction of fuel (indicated by the subscript f), H_f the heat of reaction of fuel, k the turbulent kinetic energy defined by $k \equiv \frac{1}{2}(\overline{w'^2} + \overline{v'^2} + \overline{v_\theta'^2})$ (1)

(v) Γ stands for the diffusivity. The subscript under Γ represents the entity of which diffusion has taken place.

(vi) μ_t and μ are the turbulent and laminar viscosity;

δ_H and δ_k, δ_j denote the Prandtl and Schmidt numbers for k and species j respectively; h_j is the specific enthalpy of species j .

(vii) $\dot{m}_j^{\text{III}}$ represents the volumetric consumption rate of species j .

It may be noted that the total stagnation enthalpy is used as a dependent variable in place of enthalpy in order to eliminate the necessity of evaluating the heat generation term associated with the latter. It will be shown later that some of the kinetic heating terms in equation (2.2.4) will disappear as well when certain assumptions concerning the transport properties are introduced. The species conservation equation (2.2.5) does not in itself completely specify the problem. The completion will depend upon the true representation of the mixture constituents which, in the present study consist of fuel, oxygen, nitrogen, carbon-dioxide and steam. Thus the following five equations of the same form as (2.2.5) may be written, one for each species, as follows:

$$\text{fuel: } \frac{\partial}{\partial t}(\rho m_f) + \frac{\partial}{\partial z}(\rho W m_f) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V m_f) = \frac{\partial}{\partial z}(\Gamma_f \frac{\partial m_f}{\partial z}) + \frac{1}{r} \frac{\partial}{\partial r}(r \Gamma_f \frac{\partial m_f}{\partial r}) + \dot{m}_f^{\text{III}} \quad (2.2.7)$$

(1) See section 2.5.1

$$\text{oxygen: } \frac{\partial}{\partial t}(\rho m_{O_2}) + \frac{\partial}{\partial z}(\rho W m_{O_2}) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V m_{O_2}) = \frac{\partial}{\partial z} \left(\Gamma_{O_2} \frac{\partial m_{O_2}}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \Gamma_{O_2} \frac{\partial m_{O_2}}{\partial r} \right) + \dot{m}_{O_2}''' \quad (2.2.8)$$

$$\text{nitrogen: } \frac{\partial}{\partial t}(\rho m_{N_2}) + \frac{\partial}{\partial z}(\rho W m_{N_2}) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V m_{N_2}) = \frac{\partial}{\partial z} \left(\Gamma_{N_2} \frac{\partial m_{N_2}}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \Gamma_{N_2} \frac{\partial m_{N_2}}{\partial r} \right) + \dot{m}_{N_2}''' \quad (2.2.9)$$

$$\text{carbon-dioxide: } \frac{\partial}{\partial t}(\rho m_{CO_2}) + \frac{\partial}{\partial z}(\rho W m_{CO_2}) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V m_{CO_2}) = \frac{\partial}{\partial z} \left(\Gamma_{CO_2} \frac{\partial m_{CO_2}}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \Gamma_{CO_2} \frac{\partial m_{CO_2}}{\partial r} \right) + \dot{m}_{CO_2}''' \quad (2.2.10)$$

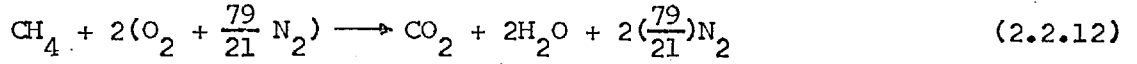
$$\text{steam: } \frac{\partial}{\partial t}(\rho m_{H_2O}) + \frac{\partial}{\partial z}(\rho W m_{H_2O}) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V m_{H_2O}) = \frac{\partial}{\partial z} \left(\Gamma_{H_2O} \frac{\partial m_{H_2O}}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \Gamma_{H_2O} \frac{\partial m_{H_2O}}{\partial r} \right) + \dot{m}_{H_2O}''' \quad (2.2.11)$$

It is however not necessary to solve all these five equations. The species continuity equation (i.e. $\sum_j m_j = 1$) may be invoked to replace one of them. The obvious choice for the replacement seems to be that of nitrogen, as its mass fraction is the largest of all of the constituents and any truncation error resulting from the numerical solution of its conservation equation would have a much pronounced effect on the accurate determination of the other species concentrations.

The species conservation set of equations may be further reduced if stoichiometric chemical reaction is assumed. In the present investigation fuel and oxidant react according to the following single-step model:

fuel + oxygen (+ nitrogen) $\longrightarrow$ products

For the methane-air reaction, the single-step model is represented by:



and the stoichiometric relations between various species may be expressed as:

$$\dot{m}_{\text{O}_2} = i \dot{m}_f \quad (2.2.13)$$

$$\dot{m}_{\text{CO}_2} = i' \dot{m}_f \quad (2.2.14)$$

$$\dot{m}_{\text{H}_2\text{O}} = i'' \dot{m}_{\text{CO}_2} \quad (2.2.15)$$

where i , i' and i'' are stoichiometric fractions.

The species conservation equations for fuel (2.2.7), oxygen (2.2.8) and carbon-dioxide(2.2.10) may be combined in pairs to form two new differential equations with two new dependent variables β and γ defined as:

$$\beta = m_{\text{O}_2} - i m_f \quad (2.2.16)$$

$$\gamma = m_{\text{CO}_2} + i' m_f \quad (2.2.17)$$

If the Schmidt numbers of all species are assumed to be equal, which is quite reasonable for turbulent flows, the individual volumetric consumption rate terms may be eliminated by the substitution of the above stoichiometric relations.

It follows that the new equations will be very similar to their original counterparts except the disappearance of the reaction rate terms,

i.e.:

$$\frac{\partial}{\partial t}(\rho\beta) + \frac{\partial}{\partial z}(\rho W\beta) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V\beta) = \frac{\partial}{\partial z}\left(\Gamma_{\beta} \frac{\partial \beta}{\partial z}\right) + \frac{1}{r} \frac{\partial}{\partial r}\left(r \Gamma_{\beta} \frac{\partial \beta}{\partial r}\right) \quad (2.2.18)$$

$$\frac{\partial}{\partial t}(\rho Y) + \frac{\partial}{\partial z}(\rho W Y) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V Y) = \frac{\partial}{\partial z}\left(\Gamma_Y \frac{\partial Y}{\partial z}\right) + \frac{1}{r} \frac{\partial}{\partial r}\left(r \Gamma_Y \frac{\partial Y}{\partial r}\right) \quad (2.2.19)$$

Not only are the two differential equations having the same form, but in the present problem they also possess the same type of boundary conditions. In such a case, only one of them, say the equation(2.2.18), needs to be solved and the other can be replaced by the following linear algebraic expressions:

$$Y = Y_1 + \frac{Y_2 - Y_1}{\beta_2 - \beta_1} (\beta - \beta_1) \quad (2.2.20)$$

where subscripts 1 and 2 represent the two positions along the boundaries in which the values of Y and β are known.

Consider the species conservation equations for steam(2.2.11) and for carbon-dioxide(2.2.10) both of which satisfy a similar set of boundary conditions. They can be made identical provided that equation (2.2.15) and the following relationship are substituted into one of them, viz:

$$m_{H_2O} = i'' m_{CO_2} \quad (2.2.21)$$

Thus this expression is used to replace the steam conservation equation.

In summarising, four of the five equations given by (2.2.7) to (2.2.11) have now been replaced by one differential equation with new dependent variables and three algebraic expressions leaving only the fuel conservation equations to be solved in its original form. The final set of the species conservation equations now appears as follows:

$$\frac{\partial}{\partial t}(\rho m_f) + \frac{\partial}{\partial z}(\rho W m_f) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V m_f) = \frac{\partial}{\partial z} \left(\Gamma_f \frac{\partial m_f}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \Gamma_f \frac{\partial m_f}{\partial r} \right) + \dot{m}_f''' \quad (2.2.20)$$

$$\frac{\partial}{\partial t}(\rho \beta) + \frac{\partial}{\partial z}(\rho W \beta) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V \beta) = \frac{\partial}{\partial z} \left(\Gamma_\beta \frac{\partial \beta}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \Gamma_\beta \frac{\partial \beta}{\partial r} \right) \quad (2.2.23)$$

where $\beta = m_{O_2} - i m_f$

$$\gamma = \gamma_1 + \frac{\gamma_2 - \gamma_1}{\beta_2 - \beta_1} (\beta - \beta_1) \quad (2.2.24)$$

where $\gamma = m_{CO_2} + i' m_f$

$$m_{H_2O} = i'' m_{CO_2} \quad (2.2.25)$$

$$m_{N_2} = 1 - m_f - m_{O_2} - m_{CO_2} - m_{H_2O} \quad (2.2.26)$$

The set can be further simplified, for the present investigation, as follows:

(i) A hot starting jet injecting into cold air

The fuel conservation equation is replaced by the algebraic relationship $m_f = 0$.

(ii) A hot starting jet injecting into inflammable surroundings

If the mixture contents of the surroundings are the same as those originally stored inside the cylinder, β may be treated as being constant and its conservation equation need not be solved. On the other hand, should the two mixture contents be different, the solution of the full set will be required.

2.3 Turbulence model, the transport and thermodynamic properties

2.3.1 Introductory remarks

Before the differential equations can be solved, additional information is required to evaluate the stress terms $\tau_{1,1}$, $\tau_{1,2}$, $\tau_{2,2}$ and $\tau_{3,3}$ appearing in the momentum equations and their related quantities, viz. μ_t , μ , Γ 's and δ 's appearing in the other conservation equations. These stresses can be either related to other calculable quantities or obtained from the solution of additional differential equations which express their conservation. The choice here depends mainly on the state of art rather than merit. Thus the former approach is adopted in the present problem

Following an early proposal by Boussinesq (1877), who introduced the concept of effective viscosity (μ_{eff}), the stress terms may be represented by the following relationships:

$$\tau_{1,2} = \tau_{2,1} = - \mu_{\text{eff}} \left(\frac{\partial W}{\partial r} + \frac{\partial V}{\partial z} \right) \quad (2.3.1)$$

$$\tau_{1,1} = - \mu_{\text{eff}} \left[2 \frac{\partial W}{\partial z} - \frac{2}{3} \text{div } \bar{V} \right] \quad (2.3.2)$$

$$\tau_{2,2} = - \mu_{\text{eff}} \left[2 \frac{\partial V}{\partial r} - \frac{2}{3} \text{div } \bar{V} \right] \quad (2.3.3)$$

$$\tau_{3,3} = - \mu_{\text{eff}} \left[\frac{2V}{r} - \frac{2}{3} \text{div } \bar{V} \right] \quad (2.3.4)$$

where, $\text{div } \bar{V} = \frac{\partial W}{\partial z} + \frac{1}{r} \frac{\partial(rv)}{\partial r}$

and $\mu_{\text{eff}} = \mu_t + \mu \quad (2.3.5)$

The substitution of the above equations into momentum equations

yields:

$$\frac{\partial(\rho W)}{\partial t} + \frac{\partial(\rho W^2)}{\partial z} + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V W) = \frac{\partial}{\partial z}(\mu_{\text{eff}} \frac{\partial W}{\partial z}) + \frac{1}{r} \frac{\partial}{\partial r}(r \mu_{\text{eff}} \frac{\partial W}{\partial r}) - \frac{\partial P_{\text{eff}}}{\partial z} \quad (2.3.6)$$

$$\frac{\partial(\rho V)}{\partial t} + \frac{\partial(\rho V W)}{\partial z} + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V^2) = \frac{\partial}{\partial z}(\mu_{\text{eff}} \frac{\partial V}{\partial z}) + \frac{1}{r} \frac{\partial}{\partial r}(r \mu_{\text{eff}} \frac{\partial V}{\partial r}) - \frac{\mu_{\text{eff}} V}{r^2} - \frac{\partial P_{\text{eff}}}{\partial r} \quad (2.3.7)$$

where $P_{\text{eff}} \equiv P + \frac{2}{3} \mu_{\text{eff}} \text{div } \bar{V} \approx P$ (as $P \gg \frac{2}{3} \mu_{\text{eff}} \text{div } \bar{V}$)

Thus the five unknown stresses have now been replaced by a single new unknown μ_{eff} which may be evaluated with the use of an appropriate turbulence model.

2.3.2 A two equation model of turbulence

A two equation model proposed by Launder et al (1972) has been tried for its physical feasibilities. In their model μ_{eff} is expressed as a function of two turbulent quantities, k the turbulent kinetic energy [$k \equiv \frac{1}{2}(\overline{w'^2} + \overline{v'^2} + \overline{v_\theta'^2})$], and ϵ its dissipation rate. In the expression for k , the subscript θ denotes the circumferential direction, the 'prime' symbolises the fluctuating component and the 'bar' the time-averaged value. Two Navier-Stokes type of equations, written to represent the conservations of k and ϵ , together with the continuity and momentum equations, form a close set describing turbulent motion. This model has been successfully applied to obtain good predictions for a number of steady flows, e.g. free axi-symmetrical jet [Launder et al (1972)],

flow over external flat-plate [Jones (1970)] and flow through in-line tube banks [Le Feuvre (1973)]. In order to use the model for unsteady flow, the terms expressing the dependence on time of k and ϵ are introduced into the governing equations. Consequently the variation of μ_{eff} with time is automatically taken into account. In the present investigation, the conservation equations for k and ϵ are written as:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial}{\partial z}(\rho W k) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V k) = \frac{\partial}{\partial z} \left(\frac{\mu_{\text{eff}}}{\delta_k} \frac{\partial k}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\mu_{\text{eff}}}{\delta_k} \frac{\partial k}{\partial r} \right) + G - C_D \rho \epsilon \quad (2.3.8)$$

$$\frac{\partial}{\partial t}(\rho \epsilon) + \frac{\partial}{\partial z}(\rho W \epsilon) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V \epsilon) = \frac{\partial}{\partial z} \left(\frac{\mu_{\text{eff}}}{\delta_\epsilon} \frac{\partial \epsilon}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\mu_{\text{eff}}}{\delta_\epsilon} \frac{\partial \epsilon}{\partial r} \right) + \frac{C_1 \epsilon G}{k} - \frac{C_2 \rho \epsilon^2}{k} \quad (2.3.9)$$

The last two terms in equations (2.3.8) and (2.3.9) represent the rate of generation and dissipation of the variable concerned. For example, G is the rate of generation of k by turbulent shear stress which may be defined by the following expression:

$$G = 2\mu_t \left[\left(\frac{\partial W}{\partial z} \right)^2 + \left(\frac{\partial V}{\partial r} \right)^2 + \left(\frac{V}{r} \right)^2 \right] + \mu_t \left(\frac{\partial W}{\partial r} + \frac{\partial V}{\partial z} \right)^2 \quad (2.3.10)$$

where $\mu_t = C_\mu \rho \frac{k^2}{\epsilon} \quad (2.3.11)$

All the C 's are constants and δ 's are the effective Schmidt numbers.

Following values have been assigned for them by Launder and Spalding (1973):

C_μ	C_D	δ_k	C_1	C_2	δ_ϵ
.09	1.0	1.0	1.44	1.92	1.3

2.3.3 The laminar viscosity and other transport properties

The laminar viscosity of each chemical species (μ_j) is calculated from the Sutherland Law [Goh and Ma (1972)] as follows:

$$\mu_j = \mu_{\text{ref},j} \left(\frac{T}{T_{\text{ref}}} \right)^{\frac{1}{2}} \frac{1.505}{[1 + 0.505(\frac{T_{\text{ref}}}{T})]}$$

where $\mu_{\text{ref},j}$ denotes the laminar viscosity of species j at a reference temperature T_{ref} (770°K). The laminar viscosity of a mixture is given by:

$$\mu = \sum_j m_j \mu_j \quad (2.3.13)$$

The transport properties indicated by Γ 's in the total stagnation enthalpy and the species conservation equations are expressed as the ratios of the effective viscosity to the appropriate effective Prandtl or Schmidt numbers (δ 's) i.e.:

$$\Gamma's = \frac{\mu_{\text{eff}}}{\delta's} \quad (2.3.14)$$

In turbulent flows, all the values of δ 's may be taken as being equal and for a round jet, a value of 0.5 has been recommended by Launder et al (1972). This leads to the elimination of certain kinetic heating terms from the total stagnation enthalpy leaving in equation (2.2.4):

$$\begin{aligned} \frac{\partial}{\partial t}(\rho H) + \frac{\partial}{\partial z}(\rho w H) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r v H) &= \frac{\partial}{\partial z} \left(\frac{\mu_{\text{eff}}}{\delta_H} \frac{\partial H}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\mu_{\text{eff}}}{\delta_H} \frac{\partial H}{\partial r} \right) \\ &+ \frac{\partial P}{\partial t} + \frac{\partial}{\partial z} \left[\mu_{\text{eff}} \left(1 - \frac{1}{\delta_H} \right) \frac{\partial}{\partial z} \left(\frac{w^2 + v^2}{2} \right) + \left(\frac{1}{\delta_k} - \frac{1}{\delta_H} \right) \frac{\partial k}{\partial z} \right] \end{aligned}$$

$$+ \frac{1}{r} \frac{\partial}{\partial r} [r \mu_{\text{eff}} (1 - \frac{1}{\delta_H}) \frac{\partial}{\partial r} (\frac{W^2 + V^2}{2}) + r (\frac{1}{\delta_k} - \frac{1}{\delta_H}) \frac{\partial k}{\partial r}] \quad (2.3.15)$$

The equation (2.3.14) may also be used to eliminate Γ 's from the species equation and replace them with μ_{eff} and δ 's.

2.3.4 The thermodynamic properties

The density of the mixture may be calculated from the Perfect Gas Law as follows:

$$\rho = \frac{P}{RT} \sum_j \frac{M_j}{m_j} \quad (2.3.16)$$

where M_j is the molecular weight of chemical species j and R stands for the universal gas constant.

The mean specific heat at a constant pressure of each chemical species, $C_{p,j}$ may be evaluated from the following formula.

$$C_{p,j} = X_j + Y_j T + Z_j T^2 \quad (2.3.17)$$

where X_j , Y_j and Z_j are constants derived from a second order polynomial curve fitting of the specific heat-temperature data taken from Spiers (1961). The mean specific heat (C_p) is calculated from the expression:

$$C_p = \sum_j C_{p,j} m_j \quad (2.3.18)$$

2.3.5 Wall functions

Special treatment for the shear stresses, turbulent kinetic energy and its dissipation rate is necessary in the regions near the wall due to the steep variation of these variables in such neighbourhoods. Launder and Spalding (1973), using Couette flow analysis, prescribed the V-velocity profile near the wall in the plane of the nozzle exit ($z = 0$) as:

$$\begin{aligned} \frac{V}{V_{\tau}} &= \frac{1}{.437} \ln (8.8z^+) & \text{for } z^+ > 11.63 \\ \frac{V}{V_{\tau}} &= z^+ & \text{for } z^+ \leq 11.63 \end{aligned} \quad (2.3.19)$$

where V_{τ} is the friction velocity ($V_{\tau} \equiv \frac{\tau_s}{\rho}$ with τ_s being the wall shear stress) and z^+ is related to z , the distance normal to and measured from the wall in the following manner:

$$z^+ = \frac{\rho k^{\frac{1}{2}} (C_{\mu} C_D)^{\frac{1}{4}} z}{\mu} \quad (2.3.20)$$

Assuming that the generation of the turbulent kinetic energy in the vicinity of the wall is equal to its dissipation rate, the equation (2.3.19) may be manipulated to give the following expressions for τ_s to be used in the momentum equation⁽¹⁾.

$$\begin{aligned} \tau_s &= .437 \rho k^{\frac{1}{2}} (C_{\mu} C_D)^{\frac{1}{4}} V / \ln (8.8z^+) & \text{for } z^+ > 11.63 \\ \tau_s &= \rho k^{\frac{1}{2}} (C_{\mu} C_D)^{\frac{1}{4}} V / z^+ & \text{for } z^+ \leq 11.63 \end{aligned} \quad (2.3.21)$$

(1) See Appendix A

The differential equation for turbulent kinetic energy (eqn. 2.3.8) is solved with the generation and dissipation terms being replaced as follows⁽¹⁾.

$$\text{Generation term} \quad (G) = \mu_t \left(\frac{\partial V}{\partial z} \right)^2 \quad (2.3.22)$$

Dissipation term

$$\begin{aligned} (C_D \rho \epsilon) &= \rho (C_\mu C_D)^{\frac{3}{4}} k^{\frac{3}{2}} \ln(8.8z^+) / (.437z) \quad \text{for } z^+ > 11.63 \\ (C_D \rho \epsilon) &= \rho (C_\mu C_D)^{\frac{3}{4}} k^{\frac{3}{2}} z^+ / z \quad \text{for } z^+ \leq 11.63 \end{aligned} \quad (2.3.23)$$

The value of ϵ near the wall is fixed by the following relationship:

$$\epsilon = k^{\frac{3}{2}} C_\mu^{\frac{3}{4}} / (.437 z C_D^{\frac{1}{4}}) \quad (2.3.24)$$

In the present investigation, the dissipation Schmidt number of 1.3 is chosen to satisfy the simple relationship of an assumed uniform stress-layer near the wall, i.e.:

$$\delta_\epsilon = \frac{(.437)^2 C_D^{\frac{1}{2}}}{(C_2 - C_1 C_D) C_\mu^{\frac{1}{2}}} \quad (2.3.26)$$

The detailed derivation of wall functions is given in Appendix A.

(1) See Appendix A

2.4 The chemical reaction models

2.4.1 Introductory remarks

The next important task is to provide a model for the volumetric rate of fuel consumption in the fuel conservation equation (2.2.20). In the present study, two distinct models have been used, one in which chemical kinetics is assumed to be the single controlling factor and the other where both the kinetic influence and turbulent effect are considered. The former model corresponds to the 'global' Arrhenius bi-molecular expression where the consumption rate is taken to be a function of instantaneous fuel and oxygen concentration, temperature and pressure all of which are assumed to be in perfect correlation. In turbulent reacting flows further assumption of linear relationship between the instantaneous and time-averaged values of these variables is necessary before the expression can be used. Although such assumption is not strictly correct the expression remains popular and is thus included in the present investigation. The latter model refers to the 'eddy-break-up' model proposed by Spalding (1971). In it the turbulent contribution to the reaction rate is explained in terms of two turbulent quantities, namely the time-averaged reactedness which is defined as the fraction of the time at which gases of high reaction-sensitivity is present and the dissipation of concentration fluctuations. Reaction will proceed if there are gases of high enough reactedness at the interface between the small lumps or eddies of unburned gases and hot gases. As the rate at which the eddies are formed by the successive breaking-up of large lumps of fluid into small ones is directly proportional to the dissipation rate of concentration fluctuations, the reaction rate should

also proportional to this same variable. This is the central idea of the 'eddy-break-up' model.

The dissipation rate of fluctuations is usually evaluated via other turbulent quantities, such as fuel concentration fluctuation, turbulent kinetic energy and dissipation length scale. The local fluctuation of fuel concentration may be obtained either from the solution of its conservation equation or as a result of the assumption involving its relationship with the time-averaged concentration of the local, fully-burnt or unburnt gases in the mixture. Mason (1973) in his prediction of turbulent premixed reacting boundary layer flow chose the former approach, whereas Stephenson (1972) in his theoretical investigation of turbulent Bunsen flame and Runchal (1973) in his study of combustion in duct preferred the latter. In the present computation the latter approach has been employed mainly because of its simplicity.

2.4.2 The Arrhenius bi-molecular model

The volumetric rate of fuel consumption may be obtained from the following expression:

$$\dot{m}_{f,A} = - \kappa P^2 m_f m_{O_2} T^{\frac{-3}{2}} e^{\frac{-E}{RT}} \Omega \quad (2.4.1)$$

where κ stands for the pre-exponential constant, E the activation energy and Ω the correction for the variation of equivalence ratio which is defined by $\Omega = (\frac{2}{w+1})^{2.4}$. Goh and Ma (1972) introduced the Ω function to the original Arrhenius expression in order to obtain good agreement between their predictions and experimental data for the steady-jet ignition problem.

A knowledge of both the pre-exponential constant and the activation energy is required before the expression can be used. The experimental determination of E by various workers such as Fenn and Colcote (1953), Avery and Hart (1953), Falconer and von Tiggelen (1963) reveals that the value of E depends not only on the type of fuel but also on the experimental conditions. In his analytical solution of the safe-gap mechanism, Phillips (1971) used the value of 108.86 MJ/Kg mole obtained by Fenn and Colcote. The same value of E is employed in the present prediction. It has also been found that satisfactory agreement between predicted and experimental ignition results for the present problem can be obtained with μ being set equal to $5 \times 10^4 \text{ kg m}^0 \text{ K}^{3/2} \text{ s}^{-1} \text{ N}^{-2}$.

2.4.3 The eddy break-up (EDBU) model

In this model, the rate of fuel consumption influenced by the action of local turbulence is directly proportional to the dissipation rate of the concentration fluctuations (ϵ_f), viz:

$$\dot{m}_{f,t}''' = C_R \epsilon_f \quad (2.4.2)$$

where C_R , the constant of proportionality takes the value of 1.5.

The dissipation rate is related to the r.m.s. value of the fuel concentration fluctuations (g), the turbulent kinetic energy (k) and its rate of dissipation (ϵ) in the following manner:

$$\epsilon_f = - \frac{g g \epsilon}{k} \quad (2.4.3)$$

and g is evaluated from the following relationship:

$$g = C_g \frac{k}{\epsilon} \left[\left(\frac{\partial m_f}{\partial z} \right)^2 + \left(\frac{\partial m_f}{\partial r} \right)^2 \right] \quad (2.4.4)$$

where C_g is a constant equal to 6.0.

As the mixture may be assumed to contain pockets of unburned and fully-burned gases, the following upper limits are placed on the value of g :

$$g \leq m_{f,u} - m_f \quad (2.4.5)$$

$$g \leq m_f - m_{f,b} \quad (2.4.6)$$

where $m_{f,u}$ and $m_{f,b}$ stand for the unburnt and fully-burnt values of the local fuel mass-fraction both of which may be related to the conditions in the surroundings, denoted by subscript G , as follows:

$$m_{f,u} = (m_f)_G \quad (2.4.7)$$

$$m_{f,b} = \max \left[0, (m_f)_G - \left(\frac{m_{O_2}}{i} \right)_G \right] \quad (2.4.8)$$

In the situation where chemical kinetics and local turbulence are both significant, the rate of reaction is decided by the lower value of the two rates, $\dot{m}_{f,t}^{||}$ (eqn. 2.4.2) and $\dot{m}_{f,A}^{||}$ (eqn. 2.4.1). Thus,

$$\dot{m}_f^{||} = - \min (-\dot{m}_{f,t}^{||}, -\dot{m}_{f,A}^{||}) \quad (2.4.9)$$

2.5. The initial and boundary conditions

In order to obtain the solution of the partial differential equations, both boundary and initial conditions must first be prescribed. As the set of equations are elliptic in space and parabolic in time, the knowledge of the conditions along the four spatial boundaries surrounding

the domain of solution (See Fig. 2.6.1) and at the beginning of the mixing process are essential. In the present analysis, they are expressed in (z, r, t) co ordinates as follows;

2.5.1 Boundary conditions

At the nozzle-exit section ($z = 0$)

for $r < d/2$

$$W(0, r, t) = W(t)$$

$$V(0, r, t) = 0$$

$$\frac{\partial}{\partial z} P(0, r, t) = 0$$

$$m_j(0, r, t) = (m_j)_I$$

$$T(0, r, t) = T(t)$$

for $r \geq d/2$

$$W(0, r, t) = 0$$

$$V(0, r, t) = 0$$

$$\frac{\partial}{\partial z} P(0, r, t) = 0$$

$$m_j(0, r, t) = (m_j)_G$$

$$\frac{\partial}{\partial z} T(0, r, t) = 0$$

In the above expressions d stands for the diameter of the nozzle and the two subscripts I and G indicate the conditions at the nozzle-exit and in the surroundings respectively. The profiles of W and T are deduced from the experimental measurement and expressed as functions of time. The turbulent kinetic energy (k) and its dissipation rate (ϵ) may be prescribed via the concept of turbulent intensity (α) which is defined as the ratio of the directional fluctuating velocity component to the local longitudinal mean velocity (W), i.e.:

$$\alpha_1 = \frac{w}{W}$$

$$\alpha_2 = \frac{v}{W}$$

$$\alpha_3 = \frac{v_\theta'}{W}$$

The substitution of these relationships into the definition of k yields:

$$k = \frac{1}{2}(\alpha_1^2 + \alpha_2^2 + \alpha_3^2)W^2$$

Assuming the local turbulent isotropicity, ($\alpha_1 = \alpha_2 = \alpha_3 = \alpha$) the equation may be reduced to:

$$k = \frac{3}{2} \alpha^2 W^2 \quad (2.5.1)$$

Hence, for $r < d/2$, k and ϵ are assigned the following values:

$$k(0, r, t) = \frac{3}{2} \alpha^2 [W(0, r, t)]^2 \quad (2.5.2)$$

$$\epsilon(0, r, t) = [k(0, r, t)]^{3/2} / \ell \quad (2.5.3)$$

where ℓ is the dissipation length scale related to the diameter of the nozzle by:

$$\ell = \lambda d \quad (2.5.4)$$

and λ is the length scale constant.

For $r \geq d/2$, the value of k is assumed to be .01% of k at the nozzle and ϵ is calculated in the same manner as that given by equation (2.5.3).

Along the axis of symmetry ($r = 0$)

$$V(z, 0, t) = \frac{\partial m}{\partial r}(z, 0, t) = \frac{\partial k}{\partial r}(z, 0, t) = \frac{\partial \epsilon}{\partial r}(z, 0, t) = \frac{\partial T}{\partial r}(z, 0, t) = 0$$

Along the free boundary parallel to the nozzle-exit section ($z = \infty$)

$$\left. \begin{aligned} W(\infty, r, t) &= 0 \\ V(\infty, r, t) &= 0 \end{aligned} \right\} \text{ i.e. 'no-flow' condition far ahead of the jet}$$

$$\frac{\partial m_j}{\partial z}(\infty, r, t) = \frac{\partial T}{\partial z}(\infty, r, t) = \frac{\partial k}{\partial z}(\infty, r, t) = \frac{\partial \epsilon}{\partial z}(\infty, r, t) = 0$$

Along the free boundary parallel to the jet-axis ($r = \infty$)

$$P(z, \infty, t) = \text{atmospheric pressure, } P_{\text{atm}}$$

$$\frac{\partial m_j}{\partial r}(z, \infty, t) = \frac{\partial T}{\partial r}(z, \infty, t) = \frac{\partial k}{\partial r}(z, \infty, t) = \frac{\partial \epsilon}{\partial r}(z, \infty, t) = 0$$

2.5.2 Initial conditions ($t = t_i$)

$$W(z, r, t_i) = V(z, r, t_i) = 0$$

$$m_j(z, r, t_i) = (m_j)_G$$

$$T(z, r, t_i) = T_G$$

$$k(z, r, t_i) = .0001 \quad k(0, r, t_i)$$

$$\epsilon(z, r, t_i) = [k(z, r, t_i)]^{3/2} / (\lambda d)$$

2.6 Closure

The mathematical formulation for the problem of hot starting jet mixing with cold surroundings has now been completed. The governing equations and their boundary conditions have been stated; the auxiliary information which includes the prescriptions of turbulence and chemical reaction models has been given. Listed below is the resulting set of partial differential and algebraic equations presented in the form ready to be solved by a numerical technique to be described in the next chapter. All differential equations except the continuity are translated into a general form having ϕ as the dependent variable, P_ϕ the pressure gradient influence and S_ϕ the corresponding source term. Table 2.7.1 on the next page illustrates both ϕ and P_ϕ , S_ϕ functions.

Continuity:

$$\frac{\partial \phi}{\partial t} + \frac{\partial(\rho W)}{\partial z} + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V) = 0 \quad (2.6.1)$$

General equation:

$$\frac{\partial(\rho \phi)}{\partial t} + \frac{\partial}{\partial z}(\rho W \phi) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V \phi) = \frac{\partial}{\partial z} \left(-\frac{\mu_{eff}}{\delta_\phi} \frac{\partial \phi}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\mu_{eff}}{\delta_\phi} \frac{\partial \phi}{\partial r} \right) + P_\phi + S_\phi \quad (2.6.2)$$

TABLE 2.6.1: ϕ , P_ϕ and S_ϕ of the general equation

ϕ	P_ϕ	S_ϕ
W	$-\frac{\partial P_{eff}}{\partial z}$	-
V	$-\frac{\partial P_{eff}}{\partial r}$	$-\frac{\mu_{eff} V}{r^2}$
k	-	$G - C_D \rho \epsilon$
ϵ	-	$\frac{C_1 \epsilon G}{k} - \frac{C_2 \rho \epsilon^2}{k}$
H $= C_p T + m_f H_f$ $+ \frac{1}{2}(W^2 + V^2) + k$	-	$\frac{\partial P}{\partial t} + \frac{\partial}{\partial z} [\mu_{eff} (1 - \frac{1}{\delta_H}) \frac{\partial (\frac{W^2 + V^2}{2})}{\partial z}]$ $+ (\frac{1}{\delta_k} - \frac{1}{\delta_H}) \frac{\partial k}{\partial z}]$ $+ \frac{1}{r} \frac{\partial}{\partial r} [r \mu_{eff} (1 - \frac{1}{\delta_H}) \frac{\partial (\frac{W^2 + V^2}{2})}{\partial r}] + r$ $(\frac{1}{\delta_k} - \frac{1}{\delta_H}) \frac{\partial k}{\partial r}]$
$\beta = m_{O_2} - i m_f$	-	-
m_f	-	$\dot{m}_f'''$

Algebraic equations:

$$Y = Y_1 + \frac{Y_2 - Y_1}{\beta_2 - \beta_1} \quad \text{where } Y = m_{\text{CO}_2} + i' m_f \quad (2.6.3)$$

$$m_{\text{H}_2\text{O}} = i'' m_{\text{CO}_2} \quad (2.6.4)$$

$$m_{\text{N}_2} = 1 - m_f = m_{\text{O}_2} - m_{\text{CO}_2} - m_{\text{H}_2\text{O}} \quad (2.6.5)$$

CHAPTER 3

THEORETICAL INVESTIGATION AND DISCUSSIONS

3.1 Introduction

3.1.1 Objects of the Chapter

The objects of this chapter are (i) to describe a suitable solution procedure for the set of non-linear, second order, partial-differential equations derived in chapter 2 and (ii) to apply the procedure to predict the unsteady jet mixing problem which may include ignition.

3.1.2 The approach

In order to achieve the first objective, the nature of the governing equations needs to be scrutinized more closely. The inclusion of convective and source terms into the equations has made the latter non-linear and difficult to be solved by existing analytical techniques. The dependence of temperature, concentration, turbulent kinetic energy and its dissipation rate on velocities, the modelling of chemical reaction as a function of pressure and temperature, and the linking of density and viscosity to other variables, invoke the need for these equations to be solved simultaneously. Only numerical methods can offer the solution to such a complex problem.

One of the main difficulties associating with the solution for Navier-Stokes type of equations is the treatment of the pressure gradient terms. Although the pressure is one of the principal unknowns, it does not appear as such. In fact, in order to solve for velocities in the momentum equations of the form given by (2.6.2), the pressure must be known hitherto from experimentation. The usual procedure adopted to avoid this expensive process is to eliminate the pressure gradient terms from the

systems of equations by transforming the continuity and the two momentum equations into two new partial differential equations adopting stream function and vorticity as new dependent variables. While this proposition seems attractive in its economy of computing time, it possesses many vital limitations, one of which is that the pressure cannot be recovered without certain loss of accuracy. This is very important especially in such problems as unsteady-jet flow in which the precise knowledge of pressure is essential to the understanding of the phenomenon. More serious however is the incapability of this procedure to tackle the non-uniform density cases in time-dependent flows which are the main features of the present problem.

An alternative to the stream-function-vorticity approach is to solve the equations in their original forms (2.6.1 and 2.6.2) with the two velocities and pressure as aerodynamic dependent variables. Amsden and Harlow (1970), Chorin (1968), Patankar and Spalding (1972) all employed this approach to solve three-dimensional parabolic Navier-Stokes equations. The basic idea is to obtain the first approximation to all of these variables from which subsequent suitable corrections may be made to bring them to satisfy the conservation equations. The latest version of the numerical method based on this approach was presented by Patankar and Spalding (1972). They proposed a general, non-iterative, finite-difference, marching procedure for the solution of a steady three-dimensional parabolic problem of developing laminar flow in an indefinitely long duct of square cross-section.

The inspection of the set of equations dictating the present problem of starting jets shows that they are also of three-dimensional type but with parabolic characteristics in time dimension. The earlier events will determine later happenings, but not vice-versa. This particular feature

enables the solution of the time-dependent governing equations to be obtained using the same velocity-pressure approach. Here the forward-marching in time-direction will provide the solution in the z - r plane at successive time intervals. Thus the starting-jet problem is treated as quasi-steady with an instant frozen picture depicting the flow obtained at each time-step. The finite-difference method incorporating this technique will be described in details in the next section.

3.1.3 The contents of the chapter

The chapter will start with the description of the numerical finite-difference method which has been employed in the investigation of starting-jet mixing problem. This part includes the listings of finite-difference equations and their solution procedure and the incorporation into the procedure of the effect of non-uniform density. In section 3.3, various treatments introduced to procure convergence and enhance stability of the solution are reported. Other details of computation including the discussion on grid distributions are given in section 3.4. Section 3.5 describes the tests carried out to check the numerical technique and to study the feasibility of each of the two turbulence models employed. The chapter ends with presentations and discussions of the theoretical solutions for the present problem.

3.2 The finite-difference method

3.2.1 The basic strategy

In order to lay the foundation for the understanding of the method,

an outline of its general principles are summarised and listed as follows:

- (i) Finite-difference equations are derived, one for each of the dependent variables from the governing partial differential equations (2.6.1 and 2.6.2). These equations are put into algebraic form to relate the values of variable at each point in the flow domain to those at earlier time and at surrounding points. Simultaneous solution of the equations is obtained through the use of algorithm.
- (ii) With the problem being treated as quasi-steady, the solution can be obtained at a given time by scanning through every point in the z-r plane. The forwarding-marching in a small but finite time-step will permit the predictions of future events.
- (iii) In the solution procedure for each time-step, the velocity and pressure are solved before other dependent variables, ϕ 's. The approximation of the pressure field allows velocity fields to be estimated through the use of momentum equations. Further exploitation of both momentum and continuity equations will provide the true velocity and pressure fields from which the solution for other dependent variables may be obtained.

3.2.2 Finite-difference equations

The first step to be taken in any finite-difference technique is to derive algebraic expressions to replace the partial differential equations describing the flow. In the derivation⁽¹⁾, the domain of interest is covered

(1) The details of the derivation appear in Appendix B.

with a system of grid net work as shown in the z-r plane in fig.2.6-1. Here a staggered rectangular grid illustrated in fig. 3.2-1 is chosen because this arrangement possesses many convenient features. The velocities V and W are stored at the point mid-way between grid nodes so as to make it easy for the evaluation of their convective influence to the conserved quantity in question, while pressure, P and other variables, e.g. ρ , μ_{eff} and T are stored at the nodes to enable the direct calculation of pressure gradients which affect V and W. The differential equations are integrated term by term over the control volume⁽¹⁾ which has its boundary lying midway between the adjacent grid lines as depicted in fig. 3.2-2. The resulting algebraic equations relate the values of variables at each point P to those at neighbouring nodes denoted in the figure by N,S,E,W,U and D for north, south, east, west, earlier time-step (upstream) and present time-step (downstream) respectively. Upwind difference technique together with suitable assumptions (See Appendix B) concerning the variation of variables between the nodes are introduced in the derivation. The finite-difference equations may be written in the following form:

Continuity: $C^t(\rho_{P,D} - \rho_{P,U}) + C^W[(\rho W)_E - (\rho W)_P] + C^V[(\rho V)_N - (\rho V)_P] = 0$

(3.2.1)

Momentum equations:

$$W_P = A_N^W W_N + A_S^W W_S + A_E^W W_E + A_W^W W_W + B^W + D^W (P_P - P_W) \quad (3.2.2)$$

$$V_P = A_N^V V_N + A_S^V V_S + A_E^V V_E + A_W^V V_W + B^V + D^V (P_P - P_S) \quad (3.2.3)$$

(1) Three types of control volumes are used, one for V, one for W and the other for P and ϕ 's as will be shown in Appendix B.

Equations for other dependent variables ($k, \epsilon, H, m_f, \beta$):

$$\phi_P = A_N^{\phi} \phi_N + A_S^{\phi} \phi_S + A_E^{\phi} \phi_E + A_W^{\phi} \phi_W + B^{\phi} \quad (3.2.4)$$

Here A's, B's, C's and D's are coefficients. The A's contain mass fluxes and transport properties; the B's include the convective effects resulting from the previous time-step and other source terms. The C's are areas across which the fluid flows; and the D's contain areas, mass flow rates and other geometrical quantities. In Appendix B, the detailed expressions of all these coefficients are given. The superscripts t, V, W, ϕ denote time and corresponding dependent variables associated with the coefficients.

3.2.3 Solution Procedure

Equations (3.2.1) through (3.2.4) when solved simultaneously would yield V, W, P and ϕ 's at a given time step as all the coefficients may be evaluated using its values prevailing at the previous time-step. The procedure is given as follows:

(i) The unknown pressure field is guessed and assigned a value of P^* at each grid point. The solution of the estimated velocity fields (V^* and W^*) is obtained from equations (3.2.2 and 3.2.3). These approximated velocities will not, in general, satisfy the continuity equation (3.2.1), but produce a mass source m_P at each grid point P , defined by:

$$m_P = C^T (\rho_{P,D}^* - \rho_{P,U}^*) + C^W [(\rho_W)_E^* - (\rho_W)_P^*] + C^V [(\rho_V)_N^* - (\rho_V)_P^*]$$

(3.2.5)

where ρ^* is the estimated density field.

(ii) In order to eliminate this fictitious mass source, corrections to the pressure and velocity fields are required as follows:

$$P = P^* + P'$$

$$V = V^* + V' \quad (3.2.6)$$

$$W = W^* + W'$$

The above expressions when combined with momentum equations will produce (see Appendix B) the following equations:

$$W'_P = W_P - W^*_P = D^W(P'_P - P'_W) \quad (3.2.7)$$

$$V'_P = V_P - V^*_P = D^V(P'_P - P'_S) \quad (3.2.8)$$

The substitution of the above relationships in the continuity equation (3.2.1) gives the following Poisson equation in finite-difference form:

$$P'_P = A^P_{NN}P'_N + A^P_{SS}P'_S + A^P_{EE}P'_E + A^P_{WW}P'_W + B^P \quad (3.2.9)$$

where the A's include the C's and D's; and the B incorporates the mass source, m_p .

The solution of equation (3.2.9) will produce corrections for the pressure field (eqn. 3.2.6) which will in turn enable the true velocity fields to be obtained (eqns. 3.2.7 and 3.2.8).

(iii) The distributions of P, V and W are employed to provide the solution for other dependent variables ϕ 's through the use of equation (3.2.4). Corrections are found to be unnecessary in this case

if a small time-step is taken during the forward-marching.

(iv) The finite-difference equations are solved by performing on a z-r plane two sweeps of the standard tri-diagonal matrix algorithm (TDMA), one in the r-direction and the other in the z-direction. Thus for equation (3.2.4), ϕ_E and ϕ_W are taken as constants when the sweep is in the r-direction, and ϕ_N and ϕ_S are held constant during the z-direction sweep. The sweep is done line by line until all grid points have been visited. Once the calculations have been obtained for the present time-step, the procedure is repeated for the solution at the next time-step.

(v) The introduction of P' as a new dependent variable requires the prescribed velocity boundary conditions to be converted into those representing pressure corrections. Along the boundary where velocity is constant, there will be no velocity correction, and consequently the gradient of P' normal to the boundary is zero. Along the boundary of constant pressure, P' is zero if P^* there has been previously set equal to this pressure. Thus for the present study, P' at the top free boundary, $\frac{\partial P'}{\partial z}$ along the plane of the nozzle and along the downstream free boundary and $\frac{\partial P'}{\partial r}$ on the symmetry axis, have all been given a value of zero

3.2.4 Treatment for non-uniform density flow

Special treatment must be incorporated in the derivation of equation (3.2.9) to include the effect of variable-density. By assuming that the mixture obeys the perfect gas law, the following equation of state emerges:

$$\rho^* = KP^* \quad (3.2.10)$$

$$\rho' = KP' \quad (3.2.11)$$

where ρ' represents the correction for density due to the correction for pressure (P') and K is the constant defined by:

$$K = \frac{1}{RT \sum_j \frac{m_j}{M_j}} \quad (3.2.12)$$

The use of equations (3.2.10) and (3.2.11) enables the following expressions to be written for ρ , ρW and ρV (ignoring the second order 'prime' terms):

$$\begin{aligned} \rho &= KP^* + KP' \\ \rho W &= KP^*W^* + KP^*W' + KP'W^* \\ \rho V &= KP^*V^* + KP^*V' + KP'V^* \end{aligned} \quad (3.2.13)$$

The above three terms when substituted into the continuity equation (2.6.1) will yield:

$$\frac{\partial}{\partial t}(KP^* + KP') + \frac{\partial}{\partial z}(KP^*W^* + KP^*W' + KP'W^*) + \frac{1}{r} \frac{\partial}{\partial r}[r(KP^*V^* + KP^*V' + KP'V^*)] = \quad (3.2.14)$$

This equation may be rearranged into the following form:

$$\begin{aligned} \frac{\partial}{\partial t}(KP') + \frac{\partial}{\partial z}(KP^*W') + \frac{1}{r} \frac{\partial}{\partial r}(rKP^*V') + \frac{\partial}{\partial z}(KP^*W^*) + \frac{1}{r} \frac{\partial}{\partial r}(rKP^*V^*) \\ + \frac{\partial}{\partial t}(KP^*) + \frac{\partial}{\partial z}(KP'W^*) + \frac{1}{r} \frac{\partial}{\partial r}(rKP'V^*) = 0 \end{aligned} \quad (3.2.15)$$

The Poisson equation for P' (eqn.3.2.9) is derived by the integration of equation (3.2.14) over the specified control volume ⁽¹⁾. Before it can

(1) The derivation appears in Appendix B.2.

be solved, further boundary conditions for two of the extra three terms (KP' , $KP'W^*$, $KP'V^*$ in eqn. 3.2.15 which indicate the influence of the variable density) must be presented. The exception for KP' arises because of the manner in which it has been implicitly incorporated into the equation (3.2.9). By setting KP' equal to KP'_p , the term is no longer a function of the conditions prevailing at the boundary.

As for other terms, the following boundary conditions have been assigned.

- i) along the top free boundary where the pressure is constant and requires no correction, $KP'V^*$ there are given a value of zero.
- ii) along the plane of the nozzle exit where fluid is injected into the control volume, the use of the upwind difference technique requires the entering mass flux to be specified. Therefore not only the velocity but also the density (or pressure) have to be prescribed. Consequently the term ρW in eqn. (3.2-13) can now be set equal to KP^*W^* by putting $KP'W^*$ and KP^*W' equal to zero.
- iii) along the axis of symmetry and the free boundary downstream of the nozzle where the no-flow conditions apply, $KP'V^*$ and $KP'W^*$ are respectively put to zero.

3.3.3 Treatments to procure convergence and stability of the solution

Various treatments are required to procure the solution convergence and stability. These include the linearization of source terms (Table 2.6.1), the introduction of iteration within a given time-step, the increase in the number of TDMA sweeps and the use of an improved pressure-velocity corrections relationship.

3.3.1 Linearization of source terms

Linearization in the present context involves the division of source terms(S_ϕ) into two parts, one depending upon conditions prevailing at previous time-step (S_U) and the other a function of the present time-step values of variables ($S_{P\phi}$). For example in the $k - \epsilon$ equations (Table 2.6.1), the generation terms G and $C_1 \epsilon G/k$ have been made to depend upon upstream conditions, whereas the dissipation terms $-C_D \rho \epsilon$ and $-C_2 \rho \epsilon^2/k$ have been evaluated using the present-step values. Table (3.3.1) on page 69 illustrate a linearization procedure for the governing differential equations (2.6.2).

Inspection of the table reveals one interesting point; opposite signs are given to each of the two components S_U and S_P , positive to the former and negative to the latter. This is true in most cases except for the equation of m_f where the reverse occurs as a consequence of the negative rate of fuel consumption. The negative S_P , when transferred to the opposite side of S_U in the finite-difference equation to be given in Appendix B, will become positive and help to balance the errors resulting from numerical computation. In the k -equation, the S_P part of the source terms is put into the form containing k by the substitution of ϵ by $(C_\mu \rho k^2/\mu_t)$. The extra term $\frac{\partial P}{\partial t}$ in the H -equation which has been included to indicate the unsteady motion effect is assumed to depend upon the values of P upstream. As the P' -equation (3.2.15) is different from the rest of the governing equations (2.6.2), the linearization of its source terms will be treated separately in Appendix B.2.

TABLE (3.3.1) Linearization of $S_\emptyset$

$\emptyset$	$S_\emptyset = S_U + S_P \emptyset_P$	
	S_U	S_P
W	0	0
V	0	$-\frac{\mu_{\text{eff}}}{r^2}$
k	G	$-\frac{C_D C_\mu \rho^2 k}{\mu_t}$
ϵ	$\frac{C \epsilon G}{k}$	$-\frac{C_2 \rho \epsilon}{k}$
H	$\frac{\partial p}{\partial t} + \frac{\partial}{\partial z} \left[\mu_{\text{eff}} \left(1 - \frac{1}{\delta_H} \right) \frac{\partial (w^2 + v^2)}{\partial z} \right]$ $+ \left(\frac{1}{\delta_k} - \frac{1}{\delta_H} \right) \frac{\partial k}{\partial z}$ $+ \frac{1}{r} \frac{\partial}{\partial r} \left[r \mu_{\text{eff}} \left(1 - \frac{1}{\delta_H} \right) \frac{\partial (w^2 + v^2)}{\partial r} \right]$ $+ r \left(\frac{1}{\delta_k} - \frac{1}{\delta_H} \right) \frac{\partial k}{\partial r}$	0
β	0	0
m_f	$-(\dot{m}_f^{\text{III}})_U$	$2 \left(\frac{\dot{m}_f^{\text{II}}}{m_f} \right)_D$

3.3.2 Other treatments

Even with the introduction of upwind difference technique and the proper linearization of source terms, a numerical procedure of the marching integration type when used to solve a system of non-linear differential equation often produces oscillation or divergence in the solution unless a very small step-size is employed. Bigger step-size may be used if any of the following actions is taken:

a) an iteration loop is set up within a given time-step. In the present investigation five iterations for the first few steps have been found sufficient to produce accurate and stable solution.

b) the number of sweeps of the standard TDMA in both z and r directions is increased. For the momentum and other ϕ 's equations, a single sweep is still adequate but for the pressure correction equation, three sweeps are needed as accumulated truncation errors produced by just one sweep may, after a number of time-steps, be sufficiently large to initiate divergence.

c) a more accurate relationship⁽¹⁾ proposed by Tatchell (1972) is used to link the velocity and pressure corrections. In his procedure, equations (3.2.7) and (3.2.8) are replaced by the following expressions:

$$W'_P = W_P - W_P^* = ND^W (P'_P - P'_W) \quad (3.3.1)$$

$$V'_P = V_P - V_P^* = ND^V (P'_P - P'_S)$$

where N represents the influence of the terms previously ignored in the derivation of the former two equations. Thus apart from enjoying the possibility of using bigger step-size, this technique also offers better

(1) See Appendix B.3.

prospect in terms of accuracy.

In the present investigation all of the three methods described above are employed. The saving in computing time, though not considerable, is very much appreciated especially in the numerical technique of this kind where a system comprising eight partial differential equations prescribing unsteady two-dimensional flow is required to be solved. With the same number of grid nodes, the introduction of these techniques permits the increase of time-step by one-fifth without the loss of accuracy.

3.4 Details of the computation

3.4.1 Grid distributions

One of the most important factors which influence the solution of the finite-difference equations is the distribution of grid lines in the flow domain. A systematic investigation has been carried out to determine the best arrangement both in terms of distributive patterns and number of grid lines which will give predictions that are in good agreement with experimental data and required the least computing time. Thus for a given accuracy, the distributions which enable solutions to be obtained with the smallest number of grid points and the biggest step-size will be chosen.

To investigate the grid influence, various distribution (uniform or expanding towards the boundaries) have been tried. For a particular distribution, the number of grid lines in one of the two spatial directions, say z , is increased while both those in r -direction and the time-step are kept constant until the solution is found to be insensitive to further refinement. The same procedure is performed for the grid lines

in the other direction. Having found the optimum number of grid lines for this specific arrangement, the same technique is repeated for other variations. The optimum pattern is that which, for a given accuracy, has been found to be most economical in computing time.

To determine the size of the forward time-step, the following consideration has been taken; with the previously chosen grid distributions, predictions are first obtained by using the largest step-size which give a converged solution; the step-size is reduced gradually until further reduction produces insignificant changes in solution.

In the present prediction, a non-uniform 22 x 22 grid system and a maximum time step-size of .021 milliseconds have been found sufficient to give accurate results. The grid lines in z-direction expand geometrically away from the plane of nozzle-exit with the expansion ratio of 1.1. In the r-direction they are uniform up to the wall of the nozzle but expanding thereafter in the similar manner as those in the other direction with the expansion ratio of 1.25. To enhance the possibility of stable solution, the time step has initially been given a small value of .0105 milliseconds, but this is increased by a factor of 1.1 for every forward step until the assigned maximum value of .021 milliseconds has been reached. With these specifications, predictions of the mixing process [prescribed by equations (2.6.1) through (2.6.5)] at six milliseconds after the start of the motion take approximately ten minutes of computing time on CDC 6600 machine.

3.4.2 Position of the assumed free boundaries enclosing the flow field

In the solution procedure, the domain of interest illustrated in fig. 2.6.1 is enclosed by the four boundaries, the plane containing the

nozzle exit, the axis of symmetry and two other free surfaces, one of uniform pressure and the other of zero flow. While the positions of the first two boundaries are known, the same cannot be said for those of the last two. In the present computation, uniform pressure is assumed to prevail all the time along the surface at a radial distance (r) eleven diameters away from the axis of symmetry while the boundary across which there is always no flow is fifty diameter away in z-direction from the nozzle outlet.

3.4.3 The application of wall functions

The values of various wall functions described in sub-section (2.3.5) are in the present study evaluated at grid points located next to the wall. If the variables required in the evaluation are not stored at these nodes, the arithmetic means calculated from their values at the two nearest locations will be used.

It may be noted that the use of Couette-flow model for regions close to the wall eliminates the need for a fine grid there and hence the solution procedure is made more economical. In the present computation, accurate solution may be found with the first grid line being .5 diameter away from the wall.

3.5 Tests of the numerical technique

3.5.1 Introduction

Before the prediction procedure can be employed to obtain solutions for the flow under consideration, preliminary investigations must be per-

formed to confirm its validity. In order to ensure that the time-dependent aspect of the flow has been correctly incorporated, the method is applied to solve a simple one-dimensional laminar incompressible flow around an oscillating flat plate and the results are compared with exact analytical solution. The application of a two-equation turbulence-model having k and ϵ as dependent variables to unsteady flow problem is checked by comparing predictions of the development of impulsively-starting two-dimensional, incompressible, turbulent round-jet with both theoretical and experimental evidences obtained by Ma and Ong (1971). Finally experimental data of Corrsin and Uberoi (1950) for two-dimensional, hot, round, turbulent steady jet emerging from a small orifice are employed to demonstrate the versatility of the procedure in dealing with steady as well as unsteady phenomenon. Once the procedure has been validated and a representative turbulence model has been found, the mixing process of hot starting jets with either cold air or cold explosive surroundings can be predicted.

3.5.2 Flow near an oscillating flat plate

The analytical solution for flow near an infinite flat plate which executes linear harmonic oscillations parallel to itself was reported by Schlichting (1968). After time t the velocity (V) at distance z perpendicular to the wall (see fig. 3.5.1) is given by:

$$V(z,t) = V_i e^{-\eta} \cos (nt - \eta) \quad (3.5.1)$$

where V_i denotes the velocity at the plate at the start of the motion

η is related to z and a constant k_1 by the following expression:

$$\eta = k_1 z = z \sqrt{\frac{n_0}{2\mu}} \quad (3.5.2)$$

and n is a constant.

In the analysis the boundary condition required is prescribed in terms of the fluid velocity at the wall and if no slip condition is assumed, it will be equal to that of the wall itself, i.e.:

$$V(0,t) = V_1 \cos nt \quad (3.5.3)$$

Two main adaptations are required in the employment of the procedure to predict this flow. To simulate one-dimensional plane flow condition, the length of the boundary in the direction along the plane (x) is made to be very much longer than that in the other direction (z) and the curvature effect associated with axisymmetrical flow is removed. As the flow is laminar and involves uniform-property fluid, it is dictated only by the momentum and continuity equations. Fig. 3.5.1 depicts the comparison of computed and analytical velocity profiles at two different times and excellent agreement may be observed. The fluid layer at a distance z undergoes a damped harmonic oscillation of amplitude equal to $V_1 e^{-k_1 z}$ and a phase lag equal to $k_1 z$.

3.5.3 Impulsively starting-jet (air - air injection)

Introductory remarks

Before the non-isothermal, turbulent, time-dependent, starting-jet mixing of the present problem can be considered, it is essential that a separate but closely related investigation should be carried out to find a representative turbulence model which dictates the mixing process. To

this end, two distinct turbulence models, the $k - \epsilon$ on the one hand and Schlichting's constant μ_{eff} (1968) on the other have been incorporated into the prediction procedure to obtain solutions for incompressible, uniform-property, two-dimensional isothermal impulsively starting-jets. Fig. 3.5.2 depicts the situation considered. A sudden withdrawal of a solenoid valve allows air to escape through a small nozzle of a pressure vessel of infinite capacity into an open atmosphere. The impulsively starting condition implies that the jet velocity attains its steady-state value (W_{jet}) instantaneously as shown in fig. 3.5.3. All of the following results have been obtained for $W_{\text{jet}} = 122 \text{ m/s}$ and d , the diameter of the nozzle, equals to $.0254 \text{ m}$.

Predictions with the constant effective viscosity model

Predictions of the afore-mentioned problem have been obtained by Ma and Ong (1971), using the similar-solution technique and Hengrussamee et al (1973), using the time-interval method. To describe the turbulent motion, they both followed Schlichting's proposal (1968) by assuming that μ_{eff} is constant and directly proportional to W_{jet} and d , i.e.:

$$\mu_{\text{eff}} = K_2 \rho W_{\text{jet}} d \quad (3.5.4)$$

where K_2 , the constant of proportionality is the reciprocal of the effective Reynolds number ($Re_{\text{eff}} = 69.3$ in the present problem).

Fig. 3.5.4 compares the results from these two predictions with experimental data obtained by Ma and Ong (1971) and also with the results using the present 'pressure-correction' method. To indicate the self-similarity behaviour of the flow, the variables chosen for comparison are

$W_0^{**} \xi$ against $\frac{1}{\xi^2}$ which are defined as:

$$W_0^{**} = \frac{W_0 t^{\frac{1}{2}}}{J^{\frac{1}{4}}} \quad (3.5.5)$$

$$\xi = \frac{z \rho^{\frac{1}{2}}}{(\mu_{eff} t)^{\frac{1}{2}}} \quad (3.5.6)$$

where; W_0 is the longitudinal velocity along the axis of symmetry .

J is the kinematic momentum flux at nozzle outlet calculated from the following expression:

$$J = \frac{\pi}{4} W_{jet}^2 d^2 \quad (3.5.7)$$

Shown in this figure is the experimental envelope which not only reveals the near similar nature of the flow but also supports all three predictions. These predicted profiles exhibit good agreement particularly for values of $W_0^{**} \xi$ between 0 and 40, beyond which, experimental evidence is uncertain as turbulence sets in rendering measurements difficult [Ma and Ong (1971)].

The constant effective viscosity model .vs. the k - ϵ model

Fig. 3.5.5 compares in details the differences in the development of axial velocity at a station 20 diameters from the nozzle as predicted by pressure-correction method on account of the two different turbulence

models used. While the incorporation of the $k - \epsilon$ model produces nearly the same rate of change of axial velocity with time as experimental results, the rise in velocity predicted by the constant effective viscosity model is much more gradual, the consequence of which is indicated by the corresponding larger steady-state attainment time. The predicted delay time is for both cases much shorter than the experimental one, being 4 milli-seconds against 9.5 milli-seconds. Although the steady state values achieved by both models compared well, only the $k - \epsilon$ model predicts the overshoot revealed in the experimental investigation [Ma and Ong (1971)].

The smaller rise is expected from the constant effective viscosity model because it considers the mixing rate as invariant with time. In reality, mixing would be slow initially and then increase, therefore, the model overestimates the phenomenon at first, and underestimates it later. Because of this serious shortcoming, the model will from now on be abandoned in favour of the $k - \epsilon$ one which takes full account of the time-dependence of turbulent motion and shows in the figure a much better resemblance to the real mixing process, except for the delay time which is about half of the actual. Before any attempt is made to explain the discrepancy, the accuracy of the measurements should first be scrutinized. The experiment as it has been set up produced the flow which did not correspond with the ideal impulsively-starting condition; a sudden withdrawal of the valve caused initial reverse flow in the neighbourhood of the nozzle, and 2 milliseconds was reported by Ma and Ong (1971) to elapse before the nozzle velocity attained its W_{jet} value. The extent to which this reverse-flow phenomenon might interfere with the subsequent flow development is difficult to estimate. Furthermore, any small errors resulting from inaccurate assessment of instruments' sensitivity and calibration might become significant in the measurements of this kind where

the time-scale involved was in the order of milli-seconds.

The applicability of the $k - \epsilon$ model to starting-jet flow predictions

Practical limitations alone are not responsible for discrepancies displayed in the comparison. The application of the turbulence model in the prediction procedure involves in itself some uncertainties. The model does not take into account the transition which occurs when the flow changes from laminar during the early stage of its development to fully-turbulent one at a later stage. Also the values of α and λ representing respectively the mean turbulent intensity and dissipation length scale which should have been supplied from experimental measurements as a part of boundary conditions are not known. Attempts must therefore be made to prescribe them.

Fig. 3.5.6 shows the effect on the velocity-time distribution of the variation of α and λ . A similar rate of change of velocity is achieved between 4 - 8 milliseconds for most cases except for $\alpha = .08$ and $\lambda = .312$ where the rise is less steep. This insensitivity does not extend to the overshoot occurring thereafter. The smaller the values of either α or λ , the bigger is the size of the overshoot and consequently the larger the steady-state attainment time. Such phenomenon can be explained in terms of the loss of mean kinetic energy due to viscous action which is directly proportional to the local turbulent viscosity (μ_t) and mean velocity gradients. Smaller μ_t in the flow field resulting from the prescription of smaller α or λ at the nozzle outlet means that more energy is available to drive the velocity to a larger peak value, and vice versa. Because of the lack of the measurement for the overshoot, it has been decided that the parameters which give best agreement with

experimental data of the overall velocity rise are $\alpha = .05$ and $\lambda = .312$.

Further attempts have been made to increase the predicted delay time by varying the values of constants C_μ , C_1 and C_2 in the turbulence model. However the only effect seems to be the change in the rate of velocity rise. Adjustments to grid distributions also prove to be ineffective. The employment of uniform grids instead of the expanding ones would result in the turbulent wall shear stress τ_s (which are calculated from Couette's flow analysis) being underestimated. The lowering of τ_s would enable the starting jet to develop more freely in radial direction, thus decreasing the steady-state axial-velocity to an unrealistic level.

The insensitivity of delay time to changes in the values of constants of the $k - \epsilon$ turbulence model suggests that the development of the jet during the early stage of the mixing process is controlled, not by diffusion, but by convection. One of the important parameters which affects convection is the flow velocity at the nozzle exit. Ma and Ong (1971) reported that the jet took 2 milliseconds to reach its maximum W_{jet} value, so a linear profile has been introduced to replace the impulsively-starting condition. Unfortunately this only increases the delay time only slightly and it is considered futile to employ more sophisticated profiles, as, for the most precise one, the maximum increase could only be 2 milliseconds.

To demonstrate the validity of the procedure and the $k - \epsilon$ model further predictions have been obtained for $d = .0127$ m with the same W_{jet} and Re_{eff} . Shown in fig. 3.5.7 are the comparison of experimental and predicted development of axial velocity at 20 and 30 diameters from the nozzle. For the constant effective viscosity model, inaccurate predictions for the rate of mixing is still apparent. On the other hand, for the $k - \epsilon$ model, the results at both stations compare well with

measurements in so far as the velocity rise and the values of steady-state axial velocity are concerned. As in the previous case, the predicted delay time lags behind its experimental counterpart, and more so at 30 diameters than at 20. This seems to suggest that the nearer the station is to the nozzle, the less time the flow has to adjust itself to the departure from the ideal impulsively starting conditions created by a sudden withdrawal of the solenoid valve.

Concluding Remarks

The study of the isothermal, uniform-density starting-jet phenomenon has led to establishment of the turbulence model to be employed in subsequent computations. The $k - \epsilon$ model when compared with the constant effective viscosity model provides a more accurate representation of the unsteady turbulent mixing process in so far as the rate of velocity rise is concerned. To be able to predict accurately this mixing rate is extremely important particularly in the investigation of the reactive starting-jet flow to be followed. In such a case, the possibility of ignition occurring depends entirely upon the way in which the hot jet mixes with surrounding combustible mixture. The correct computation of the mixing rate will lead to the prediction of the correct phenomenon. In the light of the foregoing analysis, the $k - \epsilon$ turbulence model is thus chosen.

3.5.4 Steady flow of axisymmetrical turbulent jet

The pressure correction method has been applied to predict the

steady flow of axisymmetric turbulent jet and the results are compared with experimental evidence of Corrsin and Uberoi (1950). The purpose of this investigation is two-fold; firstly to further illustrate the versatility of the procedure and secondly to provide better understanding to the $k - \epsilon$ turbulence model. The physical situation considered is the same as the one displayed in fig. 3.5.2 except the jet in this case is steady and non-isothermal. In the computations, the system of partial differential equations prescribing the conservation of mass, momentum, turbulent quantities (k, ϵ) and total stagnation enthalpy is solved with the use of the largest possible time step which permits stable solutions. Because of the availability of experimental data, precise prescription of boundary conditions at the nozzle outlet is possible and they are, for the present predictions, $W_{jet} = 34.9$ m/s, $T_{jet} = 573^{\circ}\text{K}$, $k_{jet} = 2.4 \times 10^{-6} W_{jet}^2$ and $d = .0254$ m. To complete the problem specification, eqn. (2.5.3) has been used to evaluate ϵ_{jet} with a constant λ being set equal to the previously-employed value of .312.

Fig. 3.5.8 depicts the comparison between predictions and measurements of the normalised velocity and temperature distributions in axial direction. Good agreement between the predicted and experimental velocity profiles indicates both the applicability of $k - \epsilon$ turbulence model and the correctness of the value of λ being employed. Highly favourable comparison of the predicted and experimental temperature distribution are on the other hand to be anticipated as it is the procurement of such agreement that determines the values of the effective Prandtl and Schmidt numbers to be 0.5. The closeness of predictions to measured results is further illustrated in fig. 3.5.9 by the plots showing axial variation of jet-width represented here by $\frac{2r_1}{d}$ with r_1 being the radial distance away from the axis of symmetry where the following

condition is satisfied:

$$\frac{T - T_G}{T_{jet} - T_G} = \frac{1}{2} \left(\frac{T_O - T_G}{T_{jet} - T_G} \right) \quad (3.5.8)$$

where T_G stand for the ambient temperature.

An important conclusion may be drawn from the above analysis and the one described in section 3.5.3 regarding the prescription of boundary conditions at the nozzle outlet involving the use of the $k - \epsilon$ turbulence model. While the mean turbulent intensity there is strongly flowdependent, the value of λ may be treated, as the comparison of the experimental evidence and predictions has revealed, to be a true constant of .312.

3.6 Presentations and discussions of theoretical solutions

3.6.1 The present problems

The general objective of this section is to present theoretical solutions which will provide an understanding to the mixing patterns of hot starting jets with either cold inflammable surroundings or atmospheric air. Ignition or non-ignition resulting from the mixing process will be distinctly demonstrated by the plots displaying in each case variations of temperature, velocity, pressure, mass fractions, and turbulent quantities with both distance and time.

In all of the cases to be investigated, the hot starting jet is formed following the ignition of a combustible mixture inside the enclosure. After the ignition, hot gases which are driven

out through a small nozzle inject into the surroundings and the mixing takes place. In the predictions the varying parameters are the concentrations of the mixture inside the cylinder before the ignition and those in the surroundings both of which are specified in term of the volume percentage. The temperature and velocity of the jet at the nozzle outlet which are required as a boundary condition in the prediction procedure are determined as functions of time from measurements to be reported in Chapter 4. The corresponding turbulent kinetic energy and dissipation rate are calculated based on the prescribed turbulent intensity (α) of 10% and a dissipation length scale constant (λ) of .312. The mass-fraction of the emerging hot gases are calculated with the assumption of the stoichiometric combustion inside the enclosure (eqn. 2.2-12).

Two chemical reaction models, the 'eddy-break-up' and the 'global' Arrhenius described earlier in section 2.4 will be separately investigated. In both models, the pre-exponential constant κ and the activation energy E are set equal to $5 \times 10^4 \text{ Kg m}^0 \text{K}^{3/2} \text{s}^{-1} \text{N}^{-2}$ and $108.86 \times 10^6 \text{ J/kg mole}$ respectively.

Other conditions which are common to all the cases are listed below:

Diameter of the orifice, d	=	3×10^{-3}	m.
Ambient pressure, P_{atm}	=	1.013×10^5	N/m^2
Ambient temperature, T_G	=	293	$^{\circ}\text{K}$
Turbulent kinetic energy across the nozzle outlet, $k(0,r,t)$	=	$\alpha^2 \times 1.5 \times [W(0,r,t)]^2$	J/kg
Turbulent kinetic energy at the surroundings, k_G	=	$10^{-4} \times k(0,r,t)$	J/kg

Dissipation rate across the nozzle

$$\text{outlet, } \epsilon(0, r, t) = [k(0, r, t)]^{3/2} / \lambda d \quad \text{J/kgs}$$

Dissipation rate at the surroundings,

$$\epsilon_G = k_G^{3/2} / \lambda d \quad \text{J/kgs.}$$

The following examples are chosen for illustrative purposes.

3.6.2. Inflammable surroundings

In the first problem, both the mixtures inside the explosion cylinder and in the surroundings consist of 9% CH₄, 22% O₂, and 69% N₂ by volume. The developments of velocity and temperature of the jet emerging from the nozzle are tabulated in Table D2 of Appendix D. The stoichiometric analysis of the mixtures results in the following specification of the species concentrations and the equivalence ratio, ω :

<u>Mass fractions at nozzle exit</u>		<u>Ambient mass fractions</u>	
$(m_F)_I$	= 0.0	$(m_F)_G$	= .052
$(m_{O_2})_I$	= .046	$(m_{O_2})_G$	= .253
$(m_{N_2})_I$	= .695	$(m_{N_2})_G$	= .695
$(m_{CO_2})_I$	= .142	$(m_{CO_2})_G$	= 0.0
$(m_{H_2O})_I$	= .117	$(m_{H_2O})_G$	= 0.0

ω , the equivalence ratio = .818

According to the experimental evidence [Phillips (1971)] which will be presented in the next chapter, the mixing process involving the same mixtures does not always result in the ignition of external mixture. The probability of ignition occurring was reported to be 50%. From a theoretical point of view, such a result can be considered as the ignition limit. In the present study, the value of κ , the pre-exponential constant in the Arrhenius expression (eqn. 2.4.1), has been adjusted to a smallest possible value which would just permit ignition within a given time indicated by Phillips' experimental data. Also, for illustrative purposes, the value of κ has been further reduced to give the results for non-ignition case.

3.6.21 Non-ignition case

The results for non-ignition case are illustrated in fig. 3.6-1 to 3.6-6 by means of contour plots showing the developments at four different time-intervals of the time-mean values of temperature, concentrations, velocity-vector, static pressure, turbulent kinetic energy and its dissipation rate and shear stress with the time being measured from the instant the spark-ignition is initiated.

i) Temperature

The inspection of isotherms drawn on the left hand side of fig. 3.6-1

reveals the way in which hot gases emerging from the nozzle share their energy with surroundings. As the jet moves gradually into the ambient atmosphere, it entrains into its main body a stream of colder fluids resulting in the rise in temperature of the latter. Because of the domination of convection over diffusion in the mixing process, the rise is more prominent in forward than in outward direction as shown in the figure where at 8 ms an isotherm of 320°K is seen to reach a location 12 diameters along the jet axis while achieving the widest width of 1.6 diameters. As time proceeds, more hot gases will come out and the jet will push further away into surroundings.

ii) Concentrations

The mixing process is better illustrated by the plot on the right hand side of the same figure depicting the distribution of normalised fuel mass-fraction from which the three distinct phases of the mixing phenomenon become apparent. Initially (8 ms) the rate of entrainment is very small and fuel, a constituent in the ambient mixture, is swept away by the emerging combustion products and nitrogen. As a result little fuel is presented near the nozzle. However, as the jet continues to draw more fuel, mixing becomes stronger and fuel concentration there begins to increase, rapidly at first (9 ms) and very slowly later on to approach steady-state (10.5 ms and 11.5 ms). Further from the nozzle, fuel remains relatively undisturbed the evidence of which is displayed by the slow-moving .95 and .80 fuel concentration contours. The left hand side of the next figure, fig. 3.6-2, shows the distribution of normalised oxygen concentration to be an exact replica of that of fuel. This is not surprising, for in the present investigation the value of β , defined as $(m_{\text{O}_2} - im_f)$, is uniform everywhere in the flow field and also the diffusion

rate is the same for both species in a turbulent flow. Consequently whatever amount of fuel is being entrained into the hot jet, an equivalent amount of oxygen will accompany them. Furthermore with the uses of a simple mathematical analysis and the linear relationship existing between β and η the latter of which represents $(m_{CO_2} + i'm_f)$, the normalised carbon-dioxide mass fraction $[\frac{m_{CO_2}}{(m_{CO_2})_I}]$ displayed on the opposite side of the figure may be shown to be equal to $[1 - \frac{m_f}{(m_f)_G}]$. In other words, at a location where there exists large concentrations of fuel and oxygen, minimal amounts of carbon-dioxide are expected, and vice versa. Thus in subsequent presentations of results for the ignition case, only the distribution of fuel concentration needs to be included.

iii) Velocity vector and static pressure

The aerodynamic behaviour of the flow is distinctly illustrated by the distributions of velocity-vector and static pressure displayed in Figs. 3.6-3 and 3.6-4 respectively. In the first figure, fluid is entrained into the jet in the region near the wall, but further downstream it is being deflected away from the jet-axis. This suggests the formation of a recirculating region which is large in size, though very weak in its strength, above the main body of the jet. As the jet moves forward with time, more fluid is entrained and consequently the size of the recirculating region is increased. However the recirculation has now lost some of its strength as indicated by the decrease in the length of velocity vector within the region. At the same time, the centre of recirculation is moving slowly away from the wall at a rate much slower than that of the jet itself. An interesting point which emerges from the comparison of this figure with that of species concentration

distributions (figs. 3.6-1 and 3.6-2) is that the recirculating region consists entirely of the ambient fluid. The static pressure variation, though very small, can be illustrated by the next plot of the distribution of lines of constant pressure difference between that of the local and atmosphere. Gradually coming out of the nozzle are alternating waves of the above-atmosphere and below-atmosphere each of which corresponds to the forward-surfing into stagnant surroundings of unsteady jet. These waves appear to lose their strength while moving away from the nozzle as indicated by the decrease with time in the peak pressure.

iv) Turbulent kinetic energy, its dissipation rate and shear stress

The distributions of turbulent kinetic energy and its dissipation rate which characterises the turbulent phenomenon in the present investigation are shown in fig. 3.6-5. They are very similar in nature; both exhibit a very steep gradient in the neighbourhood of the nozzle and have their maxima which increase in magnitude with time a little further downstream. More informative however is the next diagram in fig. 3.6-6 which shows the distribution of shear stress. The maximum shear stress may be observed near the nozzle close to the location where turbulent kinetic energy is largest. This is to be expected since the generation of turbulent kinetic energy is directly influenced by the magnitude of the shear stress. Large shear stress indicates strong mixing, the feature well supported by the earlier diagrams which display the maximum gradient of species concentration and temperature near this particular region.

3.6.22 Ignition case

With the rate of chemical reaction prescribed by the 'eddy-break-up' reaction model described earlier in Chapter 2, ignition will result as shown in the next series of figures (3.6-7 to 3.6-11). The events before 10.5 ms are excluded from the presentation because they are identical to those in the non-ignition case (figs. 3.6-1 to 3.6-6).

i) Temperature and fuel concentration

The first figure (3.6-7) displays on the left hand side the distribution of temperature and on the right hand side that of fuel concentration. At $t = 10.5$ ms, a sudden rise of temperature may be observed everywhere in the flow field with the hottest region near the jet-axis represented by a closed loop contour of 1350°K . Large amount of fuel has been consumed within this particular region the evidence of which is indicated by a rapid reduction of its concentration from .50 at 9 ms. to about .20. The sharp increase in temperature and decrease in fuel concentration which is followed by an expansion of hot gases suggest that ignition has taken place. As the flame propagates further into the unburned mixture, causing the latter to burn, further expansion and temperature rise may be observed at 11.5 ms. The expansion resulting from the propagation is near-symmetrical as indicated by the contours bulging out more in radial directions in contrast to their oblong shape of the convective-dominated non-ignition case. The very high gas temperature and very low fuel concentration imply that the reaction at that instant is very incensed.

ii) Velocity-vector and static pressure

In order to confirm the ignition phenomenon, the distribution of velocity-vector is drawn in fig. 3.6-8. At $t = 10.5$ ms, the surrounding fluid may be observed to be pushed away from the hot region by the expanding hot gases instead of being entrained into the main jet body as in the previous case. The acceleration of the expansion is very fast as indicated by a large increase in the length of velocity vector near the free boundaries between $t = 10.5$ ms and $t = 11.5$ ms. Following the expansion, the recirculating region above the jet will disappear and the static pressure will rise. The increase in pressure which is illustrated in fig. 3.6-9 is most prominent at the moment near ignition, i.e. $t = 10.5$ ms when the magnitude of the difference between static and atmospheric pressure increases by about 30 times from its corresponding value at 9 ms. As the flame propagates into the open atmosphere, the pressure will be transmitted into the surroundings and a subsequent fall in the level of pressure will follow as indicated by the diagram at $t = 11.5$ ms.

iii) Turbulent kinetic energy, its dissipation rate and shear stress

Fig. 3.6-10 displays the distributions of turbulent kinetic energy and its dissipation rate to be similar to that of the previous case except that the contours have now bulged out because of the expansion. The next figure (fig. 3.6-11) is more interesting, for it shows the occurrence of the second maximum shear stress downstream of the ignition region in addition to the one near the nozzle outlet. The same figure when compared with that in fig. 3.6-6 also indicates the fall in the value of the upstream maxima from 15 N/m^2 at $t = 9$ ms to 8 N/m^2 at 10.5 ms. Thus the consequences of ignition are the promotion of mixing downstream of the

propagating flame and the reduction in the mixing level near the nozzle exit.

3.6-23 Important features

The results of the predictions have so far been presented to convey the overall picture of the phenomenon of unsteady jet mixing which may or may not include ignition. More accurate presentations are displayed in the next series of diagrams in which the variations of temperature, concentrations, longitudinal velocity and static pressure with both distance and time will be given. In the following figures, for $t \geq 10.5$ ms., the solid line will be drawn in these diagrams to represent the non-ignition case and the dotted line the ignition case. For the events preceeding 10.5 ms, solid line will be used throughout as the results for both cases are identical.

i) Axial distributions

Figs. 3.6-12 to 3.6-15 show the plots of the values of these variables at the jet axis (denoted by subscript '0') against the distance from the nozzle exit. For non-ignition case, the temperature always decreases with distance as indicated in the first figure. With chemical reaction taking place, the temperature variation is similar to that of the previous case but only up to $t = 9$ ms. At $t = 10.5$ ms., the temperature begins to increase with distance to reach a maximum value of 1350°K at 8 diameters downstream before it starts to fall. The sudden generation of heat suggests that ignition has already occurred in that neighbourhood.

To provide a better understanding of the mixing process, the distribution of temperature should be inspected simultaneously with the species concentration profiles plotted in fig. 3.6-13. In the latter

figure, fuel may be observed to diffuse continuously from the surroundings to the centre of the developing jet. When ignition occurs, the fast burning rate of the fuel will overwhelm the comparatively much slower diffusion rate, the consequence of which is shown by a spontaneous rise in temperature and a fall in fuel concentration at the locality of ignition. As time proceeds and the flow moves further downstream, the chemical reaction becomes more intensified. After 11.5 ms fuel along the jet axis is reduced to a negligible level up to $z/d = 12$ and the corresponding temperature reaches a maximum value of 1650°K at $z/d = 14$. As for the other two species the distribution patterns displayed are confirmations of the earlier deduction (see section 3.6-21) that oxygen and fuel move together and in opposite directions to carbon-dioxide.

The general aerodynamic behaviour of the starting-jet is shown in fig. 3.6-14 in which the longitudinal velocity distribution is presented. At any given time, the velocity decreases with distance from the nozzle outlet for both ignition and non-ignition cases. However in the former case, the compressibility effect resulting from the expansion of hot gases has brought about a slight increase of velocity in the region between $z/d = 18$ to $z/d = 22$ at $t = 11.5$ ms. The same effect is responsible for the deceleration of the flow which may be observed immediately upstream of this particular region. The figure also shows that the velocity of the flow in the ignition-case is higher than its counterpart in the non-ignition case.

The next three plots (figs. 3.6-15 to 3.6-17) are more informative, for they show the axial and radial distributions of static pressure, the knowledge of which is instrumental to the understanding of the formation of the jet. In the first two figures, the development of the jet, before ignition, may be seen as the forward-surfing of successive

pressure waves and for each wave, the position of maximum pressure gradient represents the jet front. The effect of impulse which results from the sudden emission of the jet through the nozzle is most prominent in the early stage of the development. During this period the peak value of the pressure wave occurring at the location just ahead of the jet front is quite high in comparison with that at a later stage when the jet has lost some of its initial high momentum to the surroundings. The appearance of the wake region behind each jet front is an indication, as shall be seen later, of the entrainment into the jet of the ambient fluid. The pattern of the distributions is changed for the ignition case after 10.5 ms when, because of ignition, the pressure everywhere has suddenly increased to the above-atmospheric level with the maximum reaching a value approximately seven times larger than the corresponding peak value of the non-ignition case. As time proceeds, the high local pressure will be released to the open surroundings resulting in a more uniform distribution of pressure in the flow field at $t = 11.5$ ms.

ii) Radial distributions

In the attempt to explain the behaviour of the flow, the cross-stream profiles of pressure ahead and behind the jet front are shown in fig. 3.6-17 (a), for non-ignition case, across the two respective z -stations ($z/d = 12.2$ and $z/d = 6.7$). In the figure the distributions at the upstream station are shown on the dotted line and that downstream in full-line. Behind the jet front ($z/d = 6.7$), the increase in pressure with distance from the jet-axis suggests that fluid is being entrained from the high-pressure stagnant surroundings into the jet which is at a comparatively lower pressure. Ahead of the jet front ($z/d = 12.2$), the opposite distribution pattern may be observed and as a consequence fluid

is now moving away from the jet-axis to the surroundings where the pressure is lower, the behaviour which indicates the presence of stagnation point nearby. The cross-stream distribution of pressure gradient shown in the same figure is a further confirmation of the phenomena just explained. For ignition case ($t = 10.5$ ms), the profiles drawn across the same two z-stations in fig. 3.6-17 (b) show that the pressure always decreases in the radial direction and therefore the outward flow into the surroundings is observed at both stations.

The difference in the ignition and non-ignition phenomena may be further illustrated by the next series of figures (3.6-18 to 3.6-20) which depict the cross-stream profiles of other dependent variables at a station 14.25 diameter away from the nozzle outlet. The first two figures illustrate respectively the decrease of temperature and the increase in fuel concentration with the cross-stream distance at all time-intervals. At 10.5 ms, when ignition has already occurred, the results of the two cases are not much different because the flame which has just been initiated has not propagated this far downstream. The progress of the reaction will become apparent one milli-second later as indicated in the figure by a rapid rise in temperature and fall in the level of fuel mass-fraction. The distribution of velocity drawn in the top picture of fig. 3.6-22 is similar to that of temperature except in the appearance of small negative velocity field which indicates the formation of recirculating zone above the main jet body. However, after ignition, this recirculating zone will be quickly dispersed by the expanding hot gases as shown in the diagram. The deceleration of the flow which may be observed in the region between the jet-axis and $r/d < 1.8$ provides further evidence of the compressibility effect which has been reported in the earlier discussion of the axial distribution of velocity. No comments are required to explain the behaviour of the pressure profiles

illustrated in the bottom picture of the same figure, as they are identical to the results presented earlier in fig. 3.6-17.

iii) Variations with time

The interpretation of the results based on the axial and radial distributions of the governing dependent variables may be confirmed by an examination of the following plots which show the developments with time of the axial values of these variables at $z/d = 14.25$. The sudden increases in temperature and velocity resulting from ignition are clearly illustrated in fig. 3.6-21 and so are the decreases in fuel and oxygen concentrations and the increase in pressure in the next two figures. For non-ignition case, no such rapid changes may be observed at any stage of the jet-development. The effect of mixing in this case is shown to produce gradual rises in temperature and velocity, a decrease in fuel concentration to its steady-state value and a non-monotonic variation of pressure with time.

3.6.24 The two chemical reaction models.

The ignition phenomenon described in the previous section has been obtained with the use of the 'eddy-break-up' reaction rate model, or model (1) as it will from now on be called, in which the rate of fuel consumption is taken as the lower of the two calculated rates, the one given by the Arrhenius expression and the other derived from the consideration of turbulent effect. A parallel investigation has also been carried out to predict the same problem but with the reaction rate computed from the Arrhenius expression alone [Model (2)].

Fig. 3.6-24 illustrates the temperature distribution at three different time intervals which have been obtained using this latter

model. The comparison of the results with the corresponding contour plots presented earlier for model (1) in fig. 3.6-1 (for $t < 10$ ms) and in fig. 3.6-7 (for $t > 10.5$) reveals the following important features.

i) the identical patterns of the distribution observed before 10 ms suggest that, in the early stage of mixing process, the two reaction rates calculated from these two-models are the same. This also implies the complete domination, in model (1), of the reaction rate given by Arrhenius expression over that influenced by the eddy-break-up action during this period.

ii) ignition predicted by using model (1) occurs approximately .5 ms later than that obtained through the incorporation of model (2). If the late-ignition result of model (1) is correct, it means that the Arrhenius expression overestimates the reaction rate at high temperature. On the other hand, the delay in the start of ignition predicted by model (1) is probably caused by the failure of this model to provide a realistic interpretation of turbulent effect which sets in as the result of the increase in flow velocity.

iii) critical judgement of the two models cannot be made without embarking on the study of the events predicted after ignition has occurred. The work would involve the investigation of the flame propagation which is the subject beyond the scope of the present project. It is sufficient here to point out that the expansion of the hot gases computed using model (1) proceeds at a slower rate than that based on model (2).

iv) as the difference in ignition times of .5 ms is small and may be considered to be negligible in comparison with the whole duration of the jet-development, it may be concluded that both models predict the same mixing pattern leading to the point of ignition. Thus in so far as the present project is concerned, the uses of Arrhenius

'global' expression and 'eddy-break-up' model gives the same predicted results.

3.6.3 Atmospheric surroundings

The mixing process under investigation involves the injection into atmospheric air of hot gases resulting from the spark-ignition of 9.8%CH₄ + air inside the enclosure. The use of the mixtures which are different from those in the previous case results in the corresponding changes in temperature and velocity boundary conditions and in the concentrations of mixtures in the flow domain. While the former are given in Table D.4 of Appendix D, the latter are listed below.

Mass fractions at nozzle

$$(m_{fI}) = 0.0$$

$$(m_{CO_2I}) = 0.0$$

$$(m_{N_2I}) = .736$$

$$(m_{CO_2I}) = .136$$

$$(m_{H_2OI}) = .128$$

Ambient mass fractions

$$(m_{fG}) = 0.0$$

$$(m_{O_2G}) = .240$$

$$(m_{N_2G}) = .760$$

$$(m_{CO_2G}) = 0.0$$

$$(m_{H_2OG}) = 0.0$$

Figs. 3.6-25 to 3.6-30 display the results of the predictions by means of contour plots at different time intervals of temperature, oxygen

concentration, velocity-vector and static pressure. The mixing pattern observed is similar to that of the non-ignition case presented in the previous section. A gradual increase in temperature and velocity which is a characteristic feature of the mixing of this type is evidently illustrated. The similarity of the two cases is further supported, as shown in the figures, by the appearance of the recirculating zone above the jet and the emission of alternating waves of the above-atmospheric and below-atmospheric pressure from the nozzle.

3.6.4 Further investigation on inflammable surroundings

The conditions under which the present prediction is made are similar to those in section 3.6-2 except that the mixture consisting of 9.8%CH₄ + air now replaces atmospheric air as the external surroundings. Consequently the values of the mass fractions of the ambient mixture change to $(m_F)_G = .057$, $(m_{O_2})_G = .220$, $(m_{N_2})_G = .723$, $(m_{CO_2})_G = 0$ and $(m_{H_2O})_G = 0.0$. This problem has been chosen for the study because it represents, as will be seen later in chapter 4, the case of 100% probability of ignition which is in contrast to the earlier ignition problem where the probability is 50%.

Shown in figs. 3.6-31 to 3.6-36 are the predicted results of the distributions of temperature, fuel concentration, velocity vector and static pressure at three different time intervals starting from the moment ignition occurs. The events before 6.6 ms have been excluded from the presentation because they are similar to those of the hot jet injecting into air case. In comparison with the 50% probability ignition may be observed to start at a region slightly closer to both the centre of the jet and the nozzle exit. After ignition, the velocity-vector

diagrams of the present problem show the flow accelerating at a comparatively faster rate than that of the previous ignition case. Apart from these two basic differences, similar qualitative nature of two ignition phenomena may be observed from the comparison.

3.6.5 The influence of grid spacing and time-step

To permit the assessment of the accuracy and reliability of the predictions, two separate investigations have been carried out to determine the effect on the solutions of the following two parameters (i) the size of the forward-marching time-step and (ii) the number of grid points in the flow field. In each investigation, the concerning parameter is varied until the value of the jet front obtained from the predictions is found to be insensitive to further refinement. The final optimum grid system is derived from the inspection of the results of the two investigations.

Effect of the time-step

The present prediction procedure employs the forward-marching time-step, $(\Delta t)^t$ which increases with time by a multiple of its previous-step value, $(\Delta t)^{t-1}$, viz:

$$(\Delta t)^t = 1.1 (\Delta t)^{t-1} \quad (3.6.1)$$

$(\Delta t)^t$ is allowed to increase until it reaches a maximum value, $(\Delta t)_{\max}$, equal to twice its starting value, $(\Delta t)^0$, i.e.:

$$(\Delta t)_{\max} = 2(\Delta t)^0 \quad (3.6.2)$$

Fig. 3.6-46 displays the results of the investigation all of which have been obtained based on 484 grid-points and with $(\Delta t)_{\max}$ between .0105 and .042 ms. The solution may be considered to be insensitive to the time-step size when the decrease in the value of the jet front, z_f/d obtained between two successive reductions of $(\Delta t)_{\max}$ is less than 4%. Thus from the figure, the grid-dependent solution may be taken as $z_f/d = 18.8$ and with $(\Delta t)_{\max} = .021$ ms.

Effect of grid spacing

The predicted results depend on not only the size of the time-step but also on the fineness of the grid spacing in the two-spatial directions, z and r . The employment of the same number of grid lines in both of these directions allows the investigation to be directed towards finding the effect of the total number of grid points on the solution. The results depicted in fig. 3.6-47 show the variation of z_f/d with this parameter for a given $(\Delta t)_{\max}$ (.021 ms) and grid distribution, the latter of which has already been described in section 3.4. Using the same criterion as that of the time-step study, the solution insensitive to the grid spacing is observed to be $z_f/d = 18.8$ obtained with 484 grid points.

The optimum specification

The inspection of the two results reveals that, from the consideration of both accuracy and economy of the computations, the optimum predictions may be obtained with the number of grid points equal to 484 (or 22 x 22 grid lines) and with $(\Delta t)_{\max}$ of .021 ms. About ten minutes of computing time on CDC 6600 machine is required for predictions

of the mixing process of six-milliseconds.

3.7 Closure

A finite-difference numerical method based on the pressure-correction scheme has been described and used to investigate the mixing process between hot starting jets and cold surroundings. The ignition or non-ignition phenomena resulting from the mixing has also been theoretically demonstrated. In the investigation, the factors affecting the flow have been taken to be the concentrations of the two mixtures, one inside the explosion cylinder and the other in the surroundings. In chapter 5, the predicted results will be compared with the experimental evidence which are reported in chapter 4.

CHAPTER 4

EXPERIMENTAL INVESTIGATION AND DISCUSSIONS

4.1 Introduction

4.1.1 Introductory remarks

The present experimental programme has been included to provide the boundary conditions required in the solution of the governing partial difference equations presented in Chapter 2. The scope of the study is however confined to obtaining the measurements of temperature and velocity at the nozzle exit since these conditions at other boundaries (free surfaces far remote from the nozzle exit or the symmetry-axis) are known. The results are presented as the temperature-time and velocity-time relationships which can be used directly in the prediction procedure.

Phillips (1971) carried out the experiment to determine the characteristics of the starting-jet mixing phenomenon. He obtained Schlieren photographs showing the development of the jet and the general flow patterns for both ignition and non-ignition cases. The present chapter reports his experimental findings which are relevant to the present study and the way in which they may be used to validate the prediction procedure.

4.1.2 The approach to obtain the measurements of temperature and velocity

The temperature and velocity of the hot gases injecting through a small nozzle into cold surroundings following the ignition of a gas mixture inside the enclosure depend on the following factors: (1) the

composition of the mixture inside the explosion cylinder before the ignition, (ii) the geometry and the nature of the nozzle passage and (iii) the ambient temperature and the thermal properties of the container. The first factor determines the after-ignition flame temperature and pressure inside the explosion cylinder, the second dictates the rates of heat transfer and pressure drop along the nozzle passage and the third decides the amount of heat loss to the container walls. The present experiment is restricted to the investigation of the effect of the first factor on the values of the temperature and velocity at the nozzle exit. Measurements are firstly obtained with the composition of the mixture inside the explosion cylinder being $9\%CH_4 + 22\%O_2 + 69\%N_2$ and the surroundings being air. If the flow through the nozzle is assumed to be one-dimensional, it will be possible to employ these results to calculate the developments of temperature and velocity for other cases with different mixture compositions.

In the present investigation, the measuring instruments chosen should satisfy the following basic requirements. They should not only be of sufficiently high-melting material but also robust enough to withstand the rapidly moving stream of hot gases. They should also have minimum interference on the flow emerging from the small nozzle and possess a fast enough response to follow the flow development.

The most suitable instruments used to measure rapidly varying temperature in flows of this kind are the immersion heat sensors, viz resistance thermometers and thermocouples. The working-section of the instrument is exposed to the gas stream and the signals it generates are monitored by electronic amplifiers or cathode-ray oscilloscope. Kaimakov and Tsaregorodtsev (1964) and O'dell (1970) employed the low-inertia resistance thermometers made of very fine tungsten wires

to measure the temperature of the flame and incandescent gases issuing from explosion-proof enclosures of electrical equipment. The resistance thermometer was used in preference to the thermocouple because the latter has a slower response due to the large size of its junction. This serious drawback may be removed if the junction is formed by the micro-torch flame-welding technique employed by Odidi (1974). Using a bare 40 μ m dia. Rh-Pt thermocouple made in this way in conjunction with an active filter, he was able to obtain a frequency response in order of 10 kHz in his measurements of the fluctuating temperature for a turbulent methane diffusion flame.

In comparison to the resistance thermometer, the thermocouple is simpler and more economical to use: it is less prone to oxidation at high temperature and its replacement is less costly. The tungsten-wire resistance thermometer, while enjoying better sensitivity, can be used to measure only the bulk temperature since its most sensitive working-section is not a point but a length of wire. In the present experiment, the instantaneous temperature at the nozzle exit is measured successively by three Rh-Pt thermocouples of different sizes. The results obtained are used to derive the true gas temperature.

As for the velocity measurement, none of the existing measuring instruments satisfy the afore-mentioned basic requirements. The hot-wire traversing probe which has been successfully employed by Ma and Ong (1971) to measure the development of velocity for an isothermal starting jet flow cannot withstand a temperature higher than 800°C. The use of impact tubes has not been contemplated because of their extremely poor response. The sophisticated but rather complicated laser anemometry has been excluded from the consideration because its development is still in its early stage and its application to unsteady-flow has, to

the author's knowledge, not been attempted.

An alternative approach is to derive the velocity from other measurable quantities. In the present investigation, a piezo-electric pressure transducer is employed to record the variation with time of pressure inside the explosion cylinder during the emission of hot gases through the nozzle. If the nozzle characteristics are known, the one-dimensional analysis of the flow there will provide the relationship between the pressure and the required velocity.

4.1.3 The contents of the chapter

The next section of this chapter is devoted to the general description of the apparatus which includes the flow arrangement feeding the explosion cylinder and the instrumentation required in the measurements of velocity and temperature. The experimental procedure is reported in section 4.3 and the results obtained are displayed and discussed in section 4.4. In the following section, Phillips' experimental findings which are relevant to the present investigation are presented. The final section of the chapter describes the analytical method used to obtain the developments of velocity and temperature at the nozzle exit from these experimental results.

4.2 The apparatus

4.2.1 The general arrangement

Fig. 4.2-1 illustrates schematically the general lay-out (see also plate I) of the apparatus employed in the present investigation. The apparatus may be divided into two different categories in accordance with their individual functions; the first is associated with the supply of the combustible mixture which consists of methane, oxygen and nitrogen to the explosion cylinder and the second involves the measurements of velocity and temperature of the hot gases ejecting from the cylinder after the spark-ignition.

The supplies of methane, oxygen and nitrogen are taken from each of the following three British Oxygen Company (B.O.C.) gas bottles, a commercial grade methane bottle of 220 cu.ft. capacity, an 'O₂ free' N₂ bottle of 240 cu.ft. capacity and a 'free O₂' bottle of 165 cu.ft. capacity. The pressure inside the gas-supply lines is regulated by pressure regulators. All the flow rates are metered by the commercial-type rotameters which have previously been recalibrated using a wet bubble flow meter (65 mm. dia.). The gases enter a mixer through separate conical-shaped slots and mix together at a pressure which is controlled by the conical angle of the slots. The homogeneous combustible mixture is then branched into two lines, one going to a Bunsen-flame burner and the other to the explosion cylinder. It may be seen later in section 4.3.3 that this arrangement will make it convenient for the experiment to be repeated (once the correct mixture has been obtained) by simply turning the butterfly valve on or off at the inlet to the cylinder. The pressure difference across the mixer and the mixer gauge pressure are measured by two mercury-in-glass manometers.

A Mohr clip is used to control the flow rate of the mixture into the cylinder. After the explosion cylinder has been filled, the mixture is ignited by the switch box. The temperature of the hot gases escaping through the nozzle and the cylinder pressure are measured by thermocouple probes placed at the nozzle and the piezo-electric pressure transducer fitted to the base of the cylinder. The signals from the probes and the transducer after being amplified respectively by the differential amplifier and the charge amplifier are fed into an oscilloscope and recorded by a camera. In order to protect these signals from external stray fields, co-axial leads of 50 Ω impedance are used to provide electrical connections between measuring instruments. The switch box is also employed as the external triggering mechanism for the oscilloscope.

4.2.2. The explosion cylinder

The vertically-mounted brass explosion cylinder (50 mm. inside dia., 250 mm. length) which is on loan from the Safety in Mines Research Establishment (S.M.R.E.), U.K. is shown in Plate II and III. A round-sectioned nozzle (3 mm. dia., 25 mm. length) is fitted to the centre of the cylinder top plate. The opening (9.5 mm. bore) near the top left corner of the cylinder is the inlet for the combustible mixture while the opposite opening of the same size is used only in the preliminary test to be reported in section 4.3.3. Near the bottom of the cylinder there are two other similar openings each of which is fitted with an elbow-shaped pressure release vent (15.9 mm. bore) via a 9.5 mm. connector.

To ignite the mixture inside the cylinder, the spark-gap is triggered

off by a switch-box (shown in Plate 1). Fig. 4.2.2 illustrates the electrical circuit of the latter; it consists essentially of a 'Weir' [†] 25 V. power supply type 441, two capacitors and a standard 12 V. automotive ignition coil. The power supply charges the capacitor (15000 μ F) via the 1 k Ω resistor. When the switch is depressed the charge is delivered through the primary winding of the ignition coil resulting in a large e.m.f. being induced in the secondary winding and consequently a spark across the gap. The second capacitor (.047 μ F) is used to suppress the spark across the switch when the latter is released to its original position.

4.2.3 Instrumentation

Thermocouples

The development of the temperature at the centre of the nozzle exit has been obtained with the use of three sets of specially-designed thermocouple probes. Plate II illustrates a general configuration of the probe. In the present investigation, the following thermocouples, 5% Rh-Pt - 20% Rh-Pt wires (125 μ m. dia.), 20% Rh-Pt - 40% Rh-Pt wires (100 μ m. dia.) and 20% Rh-Pt - 40%Rh-Pt wires (75 μ m. dia.), are used because of their high mechanical strength, working temperature and sensitivity. The steps taken in the construction of the thermocouples are as follows:

(i) the wires are annealed by electrical heating to relieve their residual stress.

(ii) the two junctions of the appropriate wires are joined together using a micro torch hydrogen flame [Friston and Westernborg (1965)] to

form a thermocouple of a very fine bead size.

(iii) both ends of the thermocouple are wound to the 500 μm diameter support wires of the same materials. The support wires are insulated from each other and from the atmosphere by threading through twin-bore alumina insulators.

Because of the high sensitivity of the thermocouple, the signals obtained from the probe contain not only the thermoelectric output but also the spikes generated by electrostatic discharge during the spark-ignition of the mixture inside the explosion cylinder. The latter may however be eliminated (see section on 'signal processing equipment' on page 111) by placing on top of the thermocouple probe a dummy probe made of a closed loop copper wire (1000 μm dia.). Both probes are then mounted on to a clamp with the junction of the thermocouple wires at the centre of the nozzle exit as shown in Plate II.

Pressure transducer

The present experiment employs a piezo-electric pressure transducer made of a barium titanate crystal type Mk.1 (on loan from S.M.R.E.) to measure the pressure changes inside the explosion cylinder. The crystal is housed inside a brass piece threaded to fit the hole (25.4 mm. bore) at the bottom of the cylinder. The function of the transducer is to convert mechanical measurement of pressure into a proportional electrostatic charge. The outstanding features which make this transducer suitable for the dynamic pressure measurement are its high natural frequency, a small rise time (in order of μs) and a linear output.

Signal processing equipment

The equipment which process the signals obtained from the probes employed in the temperature measurement and the pressure transducer are displayed in Plate IV. They consist of the differential amplifier (maximum amplification = 200), the 'Kistler' charge amplifier, and the 'Tektronics' dual-beam oscilloscope type 502A.

The differential amplifier is employed for two specific purposes:

- (i) to eliminate the spikes from the output of the thermocouple and
- (ii) to amplify the resulting signals. Consequently the amplifier circuit illustrated in fig. 4.2-3 may be divided into two parts. The first which consists of four $10\text{ k}\Omega$ resistors and a type 741 'Signetics N5' operational amplifier transistor performs the subtraction of the two signals received from the thermocouple and the dummy probe via the two input terminals. The output which is the actual induced thermoelectric e.m.f. is then amplified by the second part which comprises a 100Ω resistor, a $10\text{ k}\Omega$ transistor, a variable resistor and a 'type 741' transistor. A preliminary test on the differential amplifier using a signal generator type 'Advance' H.I reveals the following characteristic features:

maximum error of the subtraction circuit = 1.2%, band width of the system from d.c. to 6 kHz and a response time $\leq 10 \frac{\mu\text{s}}{\text{mv}}$.

The 'Kistler' charge amplifier, type 566 which has an upper frequency limit of 150 kHz is used to convert the electrostatic charge emitted by the piezo-electric pressure transducer into a proportional voltage. It also acts as impedance matching between extremely high output from the transducer and the relatively low input of the oscilloscope. The high output impedance requires the connection cables to be of high insulation resistance so as to prevent significant changes occurring when the cables

are shifted or moved during the operation. The use of co-axial leads with polythene insulation satisfies this requirement.

The output from the terminals of the charge and differential amplifiers are connected (as shown in Plate IV) to the 'Tektronics' dual-beam oscilloscope type 502A. Two voltage-time curves representing the variations with time of the pressure inside the explosion cylinder and the temperature at the centre of the nozzle outlet are displayed simultaneously on the screen and recorded by a 'Nikkormat' camera with a F.3.5 micro-lens on 'Ilford' films, type HP4 (A.S.A. 400).

4.3 Experimental procedure

4.3.1 The static calibration of the pressure transducer

In the calibration the two pressure release vents near the bottom of the explosion cylinder were sealed while the opening opposite the inlet was connected to a Hg-in-glass manometer. The cylinder was filled with nitrogen at various pressure levels. The corresponding signals emitted by the transducer and displayed as the voltage changes on the oscilloscope were compared with the readings on the manometer. The resulting calibration curve illustrated in fig. 4.3-1 shows the good linearity of the output which is to be expected from the piezo-electric pressure transducer.

4.3.2 A cold flow test to find the discharge coefficient of the nozzle

Introductory remarks

The following approach has been employed to calculate the development of velocity at the nozzle exit from the measurement of the variation with time of pressure inside the explosion cylinder during the unsteady discharge from the reservoir to the surroundings:

(i) By assuming the flow through the nozzle to be one-dimensional, compressible, polytropic and frictionless, the ideal nozzle velocity $[(w_{O,I})^I]$ is related to the reservoir pressure (P_c) at any instant of time by the following relationship⁽¹⁾:

$$(w_{O,I})^I = \sqrt{\frac{2\Psi}{(\Psi - 1)} \frac{P_{c,i}^{1/\Psi}}{\rho_{c,i}} (P_c^{\frac{\Psi-1}{\Psi}} - P_{atm}^{\frac{\Psi-1}{\Psi}})} \quad (4.3.1)$$

where $P_{c,i}$ and $\rho_{c,i}$ stand for the pressure and density inside the cylinder at the start of the discharge; Ψ is the polytropic exponent.

(ii) With the friction, the actual velocity may be related to the ideal velocity through the coefficient of discharge (C_d) which is defined as the ratio of the actual flow rate to the ideal flow rate. If a top-hat profile of velocity is assumed across the nozzle, the following expression results:

$$w_{O,I} = C_d (w_{O,I})^I \quad (4.3.2)$$

The test

From eqns. (4.3.1) and (4.3.2), it may be concluded that

(1) The derivation has been presented by Ong (1970)

the determination of the actual nozzle velocity requires the pre-determined value of the coefficient of discharge of the nozzle. A preliminary test was thus carried out towards this objective. In the test the explosion cylinder was filled with room-temperature nitrogen and sealed from the surroundings by the adhesive tape at the nozzle exit. The sudden removal of this tape started the discharge and caused the pressure inside the cylinder to drop continuously until equilibrium was attained as shown in the diagram on Plate V. The test was then repeated with the cylinder being filled at different pressures. The decreases in pressure with time for all tests are tabulated in Table D.1 of Appendix D.

To obtain the discharge coefficient, both the ideal and actual velocities must first be evaluated. While the former is calculated using eqn. (4.3.1) together with the assumption of isentropic flow through the nozzle ($\psi = 1.4$), the actual velocity is obtained by differentiating the equation of states⁽¹⁾ to give:

$$W_{O,I} = \frac{dP}{dt} \left(\frac{M_{N_2} V_c}{R T_{atm}} \right) \left(\frac{4}{\rho \pi d^2} \right) \quad (4.3.3)$$

where M_{N_2} represents the molecular weight of nitrogen, R the universal gas constant, V_c the volume of the explosion cylinder and T_{atm} the atmospheric temperature.

It may be observed that the above relationship is only applicable to a flow in which its temperature is invariant with time and not to the present flow where the emission of hot gases undergoes a continuous change in temperature. Fig. 4.3-2 illustrates the variation of the

(1) See Appendix C

discharge coefficient which has been derived from the test with Reynolds number, $Re(\equiv \frac{\rho^W_{O_2} I^d}{\mu})$. For the range of Re between 60 and 260, the value of C_d increases approximately from .5 to .7 with increasing Re .

To make use of these cold-flow results in the calculation of nozzle velocity of the emerging hot gases in the present problem, the following assumptions have been made: (i) C_d is a characteristic of the nozzle and depends only upon the nature and geometry of the nozzle (ii) The weak dependence of C_d upon Re suggests that the former may be treated as a constant of .60, a value which is the mean of the two limits of C_d obtained from the test.

4.3.3 Starting-jet measurements

The measurements were obtained with the prepared mixture inside the explosion cylinder consisting of 9%CH₄, 22%O₂ and 69%N₂ by volume and the surrounding mixture being air. The line pressure (P_B) was maintained at 2.5 cm of Hg above atmosphere and the difference in pressure across the mixer [$(\Delta P)_M$] was 7.5 cm of Hg. The nozzle through which the hot gases escaped following the spark-ignition was 3 m.m in diameter and 25 mm long. The temperature of the hot gases at the nozzle exit were measured successively by three Rh-Pt thermocouples of 75 μ m, 100 μ m and 125 μ m in diameter and the pressure inside the explosion cylinder was monitored by the piezo-electric pressure transducer. The following paragraphs report the details of the starting-jet procedure.

The supply of the mixture to the explosion cylinder

The supply line of each gas stream was adjusted by the control valve of the respective rotameter to give the required mixture ratio. A high pressure of 7.5 cm of Hg was applied across the mixer to promote good mixing and to ensure that the subsequent downstream feeding of the explosion cylinder, when required, did not affect the previously adjusted mixture ratio. Once the correct mixture has been obtained, it was essential to maintain the supply flowing so as to be able to repeat the experiment without having to readjust the control valves. The mixture when not fed into the cylinder was disposed of by burning with a Bunsen-flame burner. When the cylinder was being filled, a Mohr clip at the inlet entrance was adjusted to provide the suitable flow rate. The maximum permissible filling rate was that which would just keep the Bunsen flame alight.

To determine whether the cylinder was completely filled, the two openings, one near the top and the other near the bottom of the cylinder were each fitted with small pilot-flame tubes which have the outlets close to the Bunsen flame. When the mixture inside the cylinder reached the level of the particular opening, the gases emerging from there would be lit. The filling period was taken to be the time which elapsed between the opening of the inlet and the moment at which the two pilot flames became identical in length, colour and steadiness. During this test, the explosion cylinder was sealed to provide sufficient pressure to drive the mixture through the small pilot tubes.

The measurements

To measure the required temperature, the thermocouple probe was placed as closely as possible to the nozzle exit with the working-junction

at the centre of the nozzle. The pressure transducer used to indicate the changes in pressure inside the explosion cylinder was fitted to the base of the vessel. The charge amplifier was set on a long time constant mode of operation and just before it was used, the control switch was depressed to eliminate any residual charges left over from the previous measurement. The oscilloscope was set on single-sweep position and on automatic triggering facility, the latter being connected to the spark switch circuit. In this way, the temperature and pressure traces were obtained starting from the instant ignition took place. The voltage vs. time signals which were displayed simultaneously on the dual-beam oscilloscope were photographically recorded. The measurement of temperature was repeated using the other two thermocouple probes.

4.4. Presentations and discussions of experimental results

4.4.1 Presentations of results

Plates VI, VII and VIII display the measurements of temperature at the nozzle outlet obtained with the uses of 75 μm (20% - 40% Rh-Pt), 100 μm (20% - 40% Rh-Pt) and 125 μm (5% - 20% Rh-Pt) thermocouples respectively. All photographs also illustrate the variation with time of the pressure inside the explosion cylinder immediately after ignition. The agreement in the pressure development exhibited in these photographs which have been taken on different occasions indicates the reproducibility of the experimental results. For temperature measurements, the degree of reproducibility is shown by the comparison of the temperature development in plate VIII and plate IX which have been obtained from successive tests with

a 125 μ m thermocouple. Apart from the difference resulting from the doubling of time-scale in the latter photograph, the two results are identical both in terms of the rate of temperature variation and the attained peak temperature values.

4.4.2 Discussions of results

The results displayed in Plate VI, VII and VIII exhibit the following common features:

- (i) a delay of approximately 5 ms. immediately after the spark-ignition.
- (ii) a steady rise of between 5 and 19 ms for the pressure and between 5 and 25 ms for the temperature.
- (iii) a continuous decrease in both pressure and temperature thereafter.

During the 5 ms. ignition delay, there is no pressure or temperature rises and the signals monitored by the transducer and the thermocouple remain equal to their pre-ignition values. After ignition, the temperature signal may be observed to lag slightly behind the pressure signal. This lag indicates the period during which the cold mixture inside the nozzle passage is being driven out by the expanding hot gases. Thereafter, both the pressure and temperature begin to rise rapidly as the flame starts to propagate into the unburned mixture inside the explosion cylinder. This will proceed until the pressure attains its peak value of 1.5 atm. at 19 ms. Immediately afterwards, a rapid decrease in pressure may be observed following the sudden discharge of the contents of the cylinder through the two large vents near the bottom.

The temperature on the other hand continues to increase for approximately a further 6 ms. before a similar decrease takes place.

Fig. 4.4-1 displays the rise with time between 6 and 24 ms of the temperature of the ejecting hot gases at the centre of the nozzle exit which has been obtained with the use of the three thermocouples. At a given time, the sensitivity of the thermocouple is shown to be inversely proportional to the diameter of the wire - the smaller it is, the larger the value of temperature recorded and vice versa. For example, a maximum temperature of 1865°K , 1617°K and 1417°K was obtained by 75 μm , 100 μm and 125 μm thermocouples at 24 ms. respectively. From these measurements, the true temperature of the gases may be calculated using the analysis to be given in section 4.6-3.

The details of the pressure and temperature experimental results are given in Table D.2 of Appendix D.

4.4.3 Accuracy of measurements

The mixture ratio

The rotameters employed in the measurement of the flow rates of the mixture constituents can be read to an accuracy of $\pm .10$ of a division. This represents a maximum error of $\pm 2\%$ on the CH_4 reading, $\pm 5\%$ on the O_2 reading and $\pm 5\%$ on the N_2 reading. The reading on the mercury-in-glass manometer used to control the mixing pressure can be obtained with an accuracy of $\pm .001\text{ m.}$ to give the maximum error of 4%.

Temperature measurements

The accuracy specifications provided by the manufacturer for the two types of thermocouples employed in the measurements are as follows:

(i) for the 5% - 20% Rh-Pt wires, $\pm 4^{\circ}\text{C}$ over a temperature range 0 - 1700°C .

(ii) for the 20% - 40% Rh-Pt wires, $\pm 8^{\circ}\text{C}$ over a temperature range 0- 1800°C .

Reproducibility of experimental results

The reproducibility of the measurements has already been described and illustrated in section 4.4.1.

4.5 S.M.R.E. data [Phillips (1971)]

Phillips (1971), using the same equipment as the one employed in the present investigation, took Schlieren photographs of the developments of the starting jets which resulted from the mixing between hot gases emerging from the small nozzle and the surroundings. The parameters influencing the mixing were taken to be the mixture ratio of the gases inside the cylinder before the spark-ignition and the mixture ratio of the surrounding gases at the start of the mixing. In order to establish the characteristics of the starting-jet, Phillips carried out non-ignition tests in which the following mixtures were specified in terms of volume percentage:

Table 4.5.1: Experimental conditions of non-ignition tests

Case No.	Prepared mixture inside the explosion cylinder	Initial mixture in the surroundings
1	9% CH ₄ + 22% O ₂ + 69% N ₂	9% CH ₄ + 22% O ₂ + 69% N ₂
2	9.8%CH ₄ + air	air
3	9% CH ₄ + air	air
4	8% CH ₄ + air	air

The Schlieren photographs on plate X show the corresponding developments of the starting-jets at successive time-intervals with the uppermost picture set representing the results of case No. 1, the bottom set the results of case No. 4 and etc. The time indicated below each picture was measured from the instant the prepared mixture inside the enclosure is ignited. The absence of shock waves observed in all photographs confirms that the hot-jets emerge from the nozzle at sub-sonic velocity. At most stages of the development, the starting-jets exhibit a fully turbulent structure except in the first pictures of the second, third and fourth cases where there is some evidence of the flow undergoing the transition from laminar to turbulent ones. This was probably a direct consequence of the decrease in the nozzle velocity (or pressure inside the cylinder) resulting from the use of larger pressure release vents. The measurements of the pressure development inside the explosion cylinder for the last three cases which are tabulated in Table D.4 of Appendix D, confirm that the pressure obtained was smaller than that of the first case.

The non-ignition tests are relevant to the present study in the following respects: (i) the pressure measurements for the second, third and fourth cases can be used to calculate the corresponding velocity vs. time relationships which are supplied as the boundary conditions for the predictions (ii) the development of the jet front and width obtained graphically from the photographs may be employed to validate the prediction procedure. The calculation of the velocity development will be presented in section 4.6-2 and the validity of the predictions will be discussed in chapter 5.

For the ignition case, the external surroundings into which the emerging hot gases ejected, were adjusted to be of the same mixture ratio as the prepared mixture inside the cylinder. The critical case of 50% ignition probability was obtained with the experimental condition of case No. 1 in Table 4.5.1 in which both mixtures consist of 9% CH_4 , 22% O_2 and 69% N_2 by volume. The top three picture sets in plate XI illustrate the representative results. Ignition of the external mixture may be observed to take place always within ten or eleven milli-seconds after initiation of the spark inside the explosion cylinder. These Schlieren photographs also reveal the two possible positions at which ignition may occur. In most instances (shown in the first and third sets), ignition is seen as a ball of flame developing near the head of the moving jet 'about 5 to 80 mm. from the nozzle outlet'. The less typical results in the second set show ignition occurring in a vortex at the side of the jet, the position favoured by Wolfhard and Bruszk (1959). To obtain 100% probability of ignition, Phillips adjusted the two mixture ratios to be 9.8% CH_4 + air. The bottom set of pictures shows that ignition now occurs much closer to the nozzle exit and within a few milli-seconds after the hot-jet emerges. The comparison of the ignition

phenomena observed in these Schlieren photographs with those obtained from predictions will be made in chapter 5.

4.6 Evaluation of experimental results

4.6.1 Introductory remarks

The present section reports the ways in which the measurements of pressure and temperature can be used to calculate the developments of velocity and temperature at the nozzle exit. In the calculations, the following assumptions have been made:

- i) the only factor which determines the characteristics of a flow through a given nozzle of a fixed geometry is the composition of the mixture inside the explosion cylinder. In other words, the values of velocity and temperature at the nozzle outlet will be the same irrespective of the external surroundings, if the mixtures inside the cylinder are the same.
- ii) the flow of hot gases through the nozzle passage is one-dimensional and polytropic (with the polytropic exponent of 1.3).
- iii) the velocity and temperature are uniform across the nozzle exit.
- iv) the radial velocity across the nozzle exit is small in comparison with the longitudinal one and can be neglected.

Table 4.6.1 on page 124 lists all the cases to be investigated.

4.6.2 Velocity calculations

From the measured pressure development, the longitudinal velocity of the hot-jet at the nozzle exit may be calculated with the uses of

Table 4.6.1: Cases under which predictions are made

Case No.	Prepared mixture inside the explosion cylinder	Initial mixture in the surroundings	Measurements available?	
			Temperature at the nozzle exit	Pressure inside the explosion cylinder
1	9% CH ₄ + 22% O ₂ + 69% N ₂	9% CH ₄ + 22% O ₂ + 69% N ₂	YES	YES
2	9.8% CH ₄ + air	air	NO	YES*
3	9% CH ₄ + air	air	NO	YES*
4	8% CH ₄ + air	air	NO	YES*

*pressure measurements obtained by Phillips (1971)

eqns. (4.3.1) and 4.3.2) and with the discharge coefficient of the nozzle equal to .60. The results of the analysis are tabulated in Tables D.2 and D.4 of Appendix D and plotted against time in figs. 4.6-1 and 4.6-2. It may be observed that the shape of velocity curve depicted in fig. 4.6-1 resembles the pressure trace of plate VI, VII and VIII which were obtained from the present experiment. Fig. 4.6-2 shows the rise period of the velocity development which has been calculated from Phillips' measurements of pressure for cases (2-4) of Table 4.6.1.

4.6.3 Temperature calculation for case (1)

Theory

The measurements obtained from the three thermocouple probes for case (1) do not represent the actual temperature of the hot-jet. The latter may however be determined if suitable corrections are made to account for the errors caused by the presence of the probe in the flow. The errors resulting from conduction and radiation of heat along the lead wires and from the junction are usually of very small magnitude [Kaimakov and Tsaregorodtsev (1964), Odidi (1974)] and can be neglected. Thus only the effect of convection is considered in the present analysis.

Bailey (1931) and Carbon et al (1949) proposed the following convective-influenced heat balance equation to represent the response of thermocouple:

$$\frac{T_i - T_T}{T_i - T_{O,I}} = 1 - e^{-t/\theta} \quad (4.6.1)$$

where T_i is the initial temperature as indicated by the probe before the temperature change occurs.

T_T is the temperature given by the probe at time t .

$T_{O,I}$ is the actual temperature of the gas (at the nozzle exit).

Θ , the time constant indicating the transient characteristic of the probe, is defined by the following expression which involves the heat transfer coefficient (α_T), the diameter (d_T), the specific heat (C_T) and the density (ρ_T) of the thermocouple material.

$$\Theta = \frac{\rho_T d_T C_T}{\alpha_T} \quad (4.6.2)$$

From these two equations, it may be concluded that the factor affecting the measurements are the properties and size of the thermocouples and the conditions of the flow. As the present measurements were obtained from the thermocouples which possess the same properties, the thermocouple response at any given time would therefore be a function of the wire diameter only, i.e.

$$\Theta \propto d_T^b \quad (4.6.3)$$

The substitution of (4.6.3) in (4.6.1) yield;

$$\frac{T_i - T_T}{T_i - T_{O,I}} = 1 - e^{-atd_T^b} \quad (4.6.4)$$

where a is the constant of proportionality and b , an exponent.

Applications

Through the use of eqn. (4.6.4), the actual temperature of the gases ($T_{O,I}$) can now be calculated from the results obtained with the three thermocouples. At each time step, the values of T_T and d_T from each thermocouple are substituted into the equation. The resulting three algebraic expressions are then solved numerically by the N.A.G. library subroutine COSNAF (1972) to give $T_{O,I}$. The results, plotted together with the three sets of thermocouple measurements (shown in fig. 4.4-1) reveal the discrepancy due to convective heat loss from thermocouple to the surrounding fluid at each time step for each thermocouple size. As the heat loss depends on the velocity of the flow which rises with time (see fig. 4.6-1), the discrepancy will also increase with time as indicated in the figure. For example, the correction on 75 μm thermocouple reading increases from 134°C at 10 ms when the flow velocity is 58.8 m/s to 305°C at 20 ms when the flow velocity is 162.1 m/s.

4.6.4 Temperature calculations for cases (2-4)

To obtain the temperature development for cases (2-4) of Table 4.6.1, the following calculation procedure has been adopted:

- i) the velocity and temperature results of case (1) are used to establish the relationship between the average Nusselt ($\overline{Nu}$) and Reynolds ($\overline{Re}$) numbers for flow through the nozzle passage with $\overline{Nu}$ being calculated from the following expression⁽¹⁾:

(1) Details of the derivation appear in Appendix C.2.

$$\overline{Nu} = \overline{Re} \cdot \overline{Pr} \left(\frac{d}{4L} \right) \left(\frac{T_f - T_{O,I}}{T_f} \right) \quad (4.6.5)$$

where T_f represents the maximum flame temperature inside the explosion cylinder and $\overline{Pr}$, the average Prandtl number. $\overline{Re}$, $\overline{Nu}$ and $\overline{Pr}$ are evaluated based on the bulk temperature of the fluid inside the nozzle passage. The relationships are plotted in fig. 4.6-3 and tabulated in Table D.3 of Appendix D.

ii) $\overline{Re}$ corresponding to the velocity results which have already been obtained for cases (2-4) are first evaluated based on the assumed bulk temperature. The relationship obtained in (i) is then used to provide $\overline{Nu}$ for each of the calculated $\overline{Re}$. The substitutions of $\overline{Nu}$ and $\overline{Re}$ in eqn. (4.6-5) will yield the first estimation of $T_{O,I}$.

iii) step (ii) is repeated until the two successive iterations produce insignificant changes in $T_{O,I}$. The final solutions of $T_{O,I}$ for all cases are tabulated in Table D.4 of Appendix D.

The calculated temperature developments are displayed in fig. 4.6-4 covering only the period during which the temperature is rising. In the figure, the temperature at the early stages of the developments for cases (3) and (4) are also shown in dotted lines to represent results obtained by extrapolation. Such action has been found necessary because $\overline{Re}$ calculated at those particular time steps lie outside the range covered by the $\overline{Nu}$ vs. $\overline{Re}$ relationship.

4.6.5 Experimental results as boundary conditions in the prediction procedure

Before the experimental data of the developments of longitudinal velocity and temperature at the nozzle outlet can be used in the prediction

procedure, they must firstly be expressed as continuous functions of time.

Here polynomial functions are chosen to fit the data points, viz:

$$W_{O,I} = p_0 + p_1 t + p_2 t^2 + p_3 t^3 + \dots + p_s t^s \quad (4.6.5)$$

$$T_{O,I} = q_0 + q_1 t + q_2 t^2 + q_3 t^3 + \dots + q_s t^s \quad (4.6.6)$$

where p, q are the polynomial constants and s represents the order of the polynomial functions. The values of p, q and s are given at the bottom of Tables D.2 and D.4 of Appendix D.

If both the velocity and temperature are assumed to be uniform across the nozzle exit, the following expressions may be written for $r < d/2$:

$$W(O, r, t) = W_{O,I} \quad (4.6.7)$$

$$T(O, r, t) = T_{O,I} \quad (4.6.8)$$

In the prediction procedure eqns. (4.6.5) to (4.6.8) are used as boundary conditions at the plane of the nozzle exit.

CHAPTER 5

COMPARISON OF RESULTS, FURTHER DISCUSSIONS AND CONCLUSIONS

5.1 Introduction

In this chapter, comparison will be made of the theoretical results given in chapter 3 with corresponding experimental data which have been deduced from Phillips' Schlieren photographs presented in chapter 4. For non-ignition cases, the predicted values of jet-front and jet-width at successive time intervals will be compared with those obtained experimentally. The results of the comparison will allow the conclusions to be made regarding the validity and accuracy of the prediction procedure. For ignition cases, only a general qualitative assessment of the predicted results is possible because of the lack of experimental evidence.

The principal results of the present investigation will be reported. Also discussed are the capability of the numerical procedure and the feasibility of the two important physical input, i.e. the turbulence and chemical reaction models. The chapter ends with the recommendation for future exploration and conclusions of the present research.

5.2 Comparison of results

5.2.1 Non-ignition cases

Fig. 5.2-1 compares the development of the jet front (z_f) for the case in which both the prepared mixture inside the explosion cylinder and the external mixture consist of 9% CH_4 , 22% O_2 and 69% N_2 . Because of the sensitivity of the results of the mixing process to slight changes in experimental flow conditions which might occur during successive experiments, the value of z_f/d in the figure are represented, not by a

curve, but by an envelope of maximum deviation equal to ± 1.5 in z_f/d . Considering this experimental scatter and theoretical inaccuracy which may arise from the interpolation of the pressure axial distribution to obtain the jet front (i.e. the position of maximum pressure gradient), the agreement between the predicted and experiment results observed is excellent, particularly between 7 and 10 ms. Here the time is measured from the instant the spark inside the enclosure is initiated. For $t > 10$ ms., the comparison is still favourable although the rate of the development of the jet-front computed is seen to be slightly smaller than that suggested by experimental evidence.

Fig. 5.2-2 shows, for the same case, the comparison of the development of the jet width (r_w) at a station 14.25 diameter downstream of the nozzle outlet. The comparatively large discrepancy is probably a direct consequence of the manner in which the computed jet-width has been defined. The radial distance from the jet-axis to a position where temperature is 320°K obtained from predictions may not correspond to the distance to the edge of the jet measured from Schlieren photographs as the experimental jet-width. Also because the jet is a turbulent one, its edges are brush-like and cannot be measured with precision from these photographs. Nevertheless the comparison may be regarded as satisfactory.

Similar comparisons are made for the next case which involves the uses of atmospheric air as the external mixture and 9.8% CH_4 + air as the prepared mixture inside the explosion cylinder. As in the previous case, the agreement between the predicted and experimental results may be observed to be better for the development of the jet front (fig. 5.2-3) than that for the development of the jet-width (fig. 5.2-4).

The next case is similar to the previous one except that the prepared mixture inside the explosion cylinder now consists of 9% CH_4 and air

instead of 9.8% CH_4 and air. Fig. 5.2-5 illustrates the comparison of the developments of the jet front for this case. While good agreement can be observed for $t > 8.5$ ms, the results before then show the predicted front developing at a slower rate than that obtained from the experiment. The discrepancy is probably caused by the inadequacy of the turbulence model to predict accurately the flow which undergoes a transitional change from laminar at the early stage of the development when the velocity is low to fully turbulent one at a later stage. This may be further illustrated in fig. 5.2-6 which shows the comparison of the predicted and experimental jet-fronts obtained when the prepared mixture inside the explosion cylinder has been diluted to 8% CH_4 + air. The larger discrepancy than that of the previous case may be observed following the dilution which effectively decreases the velocity of the emerging jet. With respect to this minor theoretical inaccuracy, the comparisons shown in these last two figures further support the validity of the present prediction procedure for non-reacting flows.

5.2 Ignition case

The comparison of ignition phenomena obtained from predictions on the one hand and experiments on the other will be made based on the qualitative information deduced from the contour plots of the former (figs. 3.6-7 and 3.6-31) and Phillips' Schlieren photographs (Plate XI) for the latter. The prediction for the 'ignition-limit' case (i.e. 50% ignition probability) in which both the prepared mixture inside the explosion cylinder and the surrounding mixture consist of 9% CH_4 , 22% O_2 and 69% N_2 , agree with Phillips' experimental findings that ignition occurs near the centre of the jet-axis, and not at the side vortex as suggested by Wolfhard and Bruzak (1959). The predicted position at which ignition takes place (18 mm. from the nozzle exit) cannot however be verified with experimental data because of the reported large scatter of the latter. It may also be observed that this position of ignition is relatively close to the nozzle exit. This may be explained by the favourable conditions of the temperature of the jet and the concentrations of the

reactive species at that particular location.

By altering the contents of the two mixtures to 9.8% CH₄ and air, the probability of ignition could, according to Phillips, be increased to 100%. Fig. 3.6-31 illustrates that the predicted ignition has now occurred on the jet-axis at a distance approximately 3 m.m closer to the nozzle exit than that in the previous case. A similar trend is also displayed in the Schlieren photograph on plate XI. Instead of ignition taking place about 5 milliseconds after the first appearance of the hot-jet from the nozzle exit as predicted, only one or two milliseconds delay has been reported. The cause of this discrepancy is probably due to the omission of the effect of unburned combustible mixture which emerges from the nozzle ahead of the combustion products. As the duration of such emission is not known, the starting jet is assumed to consist always of combustion products only. Apart from this discrepancy, the general qualitative agreement of the two ignition phenomena may be considered to be satisfactory.

5.3 The principal results

The principal results of the present investigation may be summarized as follows:

1. A numerical procedure has now been developed for the prediction of turbulent, two-dimensional compressible, time-dependent flows.
2. The procedure has been applied to predict the development of isothermal, homogeneous turbulent, impulsively-starting jets. The turbulent motion has been prescribed using either the $k-\epsilon$ model or the constant effective viscosity model. The comparison of the predicted results with existing experimental evidence suggests the superiority of the $k-\epsilon$ model.
3. The numerical procedure with the $k-\epsilon$ turbulence model incorporated

has been successfully employed to obtain predictions of the ignition or non-ignition phenomenon which results from the mixing between a hot starting-jet issuing from a small nozzle and cold surroundings.

4. The predicted results are used to illustrate the difference between the two phenomena. The occurrence of ignition near the centre of the jet-axis is accompanied by a sudden increase in local temperature and pressure and reduction in local fuel concentration. The evidence of the propagating flame is clearly illustrated by rapid expansion of the hot gases throughout the flow field following the ignition. For non-ignition cases, the changes of these variables are much more gradual.

5. In the prediction of ignition, the rate of chemical reaction is prescribed by either the 'eddy-break-up' or the Arrhenius 'global' model. While both models predict the same flow leading to the moment of ignition, the predicted speed of the flame propagation obtained thereafter is faster when the latter model is used.

6. To demonstrate that predictions obtained are qualitatively sound for ignition cases and also quantitatively accurate for non-ignition cases, they have been compared with experimental evidence. A satisfactory agreement observed from the comparison indicates the accuracy and validity of the present prediction procedure. The exclusion of the claim for quantitative success in the prediction of ignition cases is due entirely to the limited experimental data available for a conclusive comparison.

7. An experimental investigation has been carried out to obtain the developments of the temperature and velocity at the nozzle exit (required as the boundary conditions in the prediction procedure). The results show the increases of both velocity and temperature with time, gradual at first and more rapid later on. After reaching the maxima, the values of these

variables start to fall very rapidly to the values existing before the discharge.

5.4 The capabilities of the prediction procedure

Although the present method has been originally intended for obtaining predictions, leading to ignition, of the unsteady, sub-sonic non-isothermal mixing process between two streams of fluids, it is also capable of handling the flame propagation as a consequence of ignition. But in doing so, the domain of solution must be enlarged to accommodate the propagating flame. With suitable modifications, the prediction procedure can also be extended to handle super-sonic flows provided that

- (i) the effect of shock at the nozzle exit can be prescribed and
- (ii) the grid lines there are close enough to account for the steep gradient of properties across the shock waves.

From an economy point of view, the prediction procedure will prove to be an important tool in the design of many engineering equipment. The cost of computing time (in order of 10 minutes for flows lasting approximately 10 ms) is likely to be much less than that of experimentation or model-testing. Although the present work is aimed towards establishing the foundation for the computer-aided design of the flame-proof enclosure, it can also lead to study many other practical problems such as the pilot flame ignition in supersonic ramjets and the fuel injection system in rocket and diesel engines.

5.5 Comments on the $k-\epsilon$ turbulence model

While the predictions obtained through the use of the $k-\epsilon$ model appear to be highly favourable, to say that the model is perfect suggests naivety. The discrepancy in the values of the predicted and experimental jet-front observed during the early stage of the non-reacting mixing results indicates that the model is incapable of predicting accurately the flow with transitional change from laminar to turbulence. For a fully-turbulent flow the results are far more encouraging.

Although the model has been well tested for various classes of steady flow, its application to the unsteady process is novel. Because of the lack of information, the constants and the form of the mathematical equations representing the model have not been altered except for the inclusion of the terms expressing the time-dependence of k and ϵ . With respect to all these uncertainties, the model may be considered as providing a good description of the mixing process under investigation.

5.6 Comments on the chemical reaction models

Through the use of the 'eddy-break-up' model, it is now possible to include the effect of turbulence as well as chemical-kinetics on the rate of chemical reaction. To study its feasibility, the most recent form of the model [Runchal (1973)] has been incorporated into the prediction procedure and the resulting flow patterns have been compared with those obtained from using the well-established Arrhenius 'global' model.

For the events preceeding ignition, both models give the predictions which are similar and in qualitative agreement with experimental evidence.

As the objective of the present work is to investigate the mixing leading to ignition, both models may be regarded as providing satisfactory predictions. The predicted results also indicate that the influence of chemical kinetics overrides that of turbulence during the early stage when the temperature is still low. However, after ignition the effect of turbulence becomes apparent and the speed of flame propagation predicted by the 'eddy-break-up' model is observed to be slower than that obtained by the other model. To be able to assess these results would necessitate the acquirement of more experimental data on this particular topic which is at present unavailable.

5.7 Suggestions for future research

Undoubtedly the most profitable area of the extended research is to obtain experimental data on ignition and the subsequent flame propagation so that the ability of the prediction procedure to handle these cases quantitatively may be confirmed. Provided that suitable experimental techniques are available, extensive measurements of temperature and velocity should be made at various positions in the flow field in addition to the Schlieren's photographs. These measurements will also prove to be instrumental in the attempt to improve the turbulence model employed in the present prediction procedure.

On the theoretical side, in order to eliminate the necessity of having to prescribe boundary conditions at the nozzle exit, the prediction procedure should be extended to cover the whole of the flow region including the inside of the enclosure. In this case, modifications would have to be introduced to account for the changes in boundaries enclosing the flow. Also to retain the same accuracy, the number of grid lines and consequently

the computer time must be greatly increased. The extended procedure will have a direct application in the design of flame-proof enclosure.

A simplified single-step chemical reaction assumed in the present theoretical study does not in reality represent the real combustion process. Reactions between methane and air are known to proceed to many intermediate steps forming many intermediate radicals. Before the multi-step reactions can be included to reflect the reality, though at the expense of economy, further study is firstly required into the details of the chemical kinetic mechanism of these reactions.

The author believes that the present work has provided a major step forward in the investigation of the time-dependent motion of non-uniform property fluids. Further work should aim at the exploitation of the present prediction procedure to help the design of engineering equipment in which such mixing plays a dominant role.

5.8 Conclusions

For the present investigation, the following conclusions may be drawn:

1. A calculation procedure based on the 'pressure-correction' technique has been successfully developed to predict the mixing of hot, turbulent, round-sectioned, starting jets with cold surroundings.
2. A turbulence model characterised by two differential equations representing the conservation of turbulent kinetic energy and its dissipation rate, has been found to be suitable for the predictions of the present unsteady-flows.
3. Transient flow patterns at successive time intervals predicted by the

procedure has been employed (i) to study ignition and non-ignition phenomena resulting from the mixing process and (ii) to demonstrate the difference between them.

4. The predicted results for non-ignition cases have been shown to be in good quantitative agreement with experimental evidence. For ignition cases, the comparison is not conclusive because of insufficient experimental data.

5. An experimental investigation has been carried out to determine the developments of velocity and temperature at the nozzle exit. The results are used as boundary conditions in the prediction procedure.

NOMENCLATURE

<u>Symbols</u>	<u>Meaning</u>	<u>Equation of first mention</u>
a	proportional constant in the calculation of time constant of thermocouple	eqn. (4.6.4)
b	exponential constant in the calculation of time constant of thermocouple	eqn. (4.6.3)
A,B,C,D	coefficients in the general finite-difference equation for ϕ 's	sec. 3.2.2
C_1, C_2, C_D, C_μ	constants of the $k - \epsilon$ turbulence model	eqns. (2.3.8-11)
C_g, C_R	constants of the 'eddy-break-up' model	eqns. (2.4.2-4)
C_p	specific heat at a constant pressure of the mixture	eqn. (2.2.6)
C_T	specific heat at a constant pressure of thermocouple	eqn. (4.6.2)
C_p	coefficient of discharge of the nozzle	eqn. (4.3.2)
d	nozzle diameter	sec. (2.5.1)
div	divergence - a vector operator	eqn. (2.3.2)
E	activation energy in Arrhenius expression	eqn. (2.4.1)
F	coefficient in the general finite-difference equation for ϕ 's	eqn. (B.3)
g	r.m.s of fuel concentration fluctuations	eqn. (2.4.3)
G	generation of turbulent kinetic energy	eqn. (2.3.8)
G^r, G^z	terms associated with diffusion in the finite-difference equation for the pressure-correction	eqns. (B.22, B.23)

<u>Symbols</u>	<u>Meaning</u>	<u>Equation of first mention</u>
h	specific enthalpy	eqn. (2.2.4)
H	total stagnation enthalpy	eqn. (2.2.4)
H_f	heat of reaction	eqn. (2.2.6)
i, i', i''	stoichiometric fractions	eqns. (2.2.13-15)
J	kinematic momentum flux at nozzle outlet	eqn. (3.6.5)
k	turbulent kinetic energy	eqn. (2.2.4)
k_1	constant associated with flow near oscillating flat plate	eqn. (3.5.2)
k_g	thermal conductivity of the mixture	eqn. (C.2.2)
K	constant of the perfect gas law	eqn. (3.2.10)
K_2	constant associated with Schlichting's constant effective viscosity model	eqn. (3.5.4)
l	dissipation length scale	eqn. (2.5.3)
l_N	length of the nozzle passage	eqn. (C.2.1)
L	mixing length	eqn. (A.17)
L^r, L^z	terms associated with convection in the general finite-difference equation for ϕ 's	eqn. (B.3)
m	species concentration	eqn. (2.2.4)
m_c	mass of the contents of the explosion cylinder	eqn. (C.1.1)
m_p	mass source at the point P	eqn. (3.2.5)
$\dot{m}$	volumetric rate of consumption	eqn. (2.2.5)
M	molecular weight	eqn. (2.3.16)
n	constant associated with flow near oscillating flat plate	eqn. (3.5.1)

<u>Symbols</u>	<u>Meaning</u>	<u>Equation of first mention</u>
N	factor in the improved finite-difference momentum equation	eqn. (3.3.1)
$\overline{Nu}$	average Nusselt number of flow through the nozzle	sec. (4.6-4) eqns.(4.6.5-6)
P,q	coefficients in the expressions for velo- city and temperature at the nozzle outlet	eqns.(4.6.5-6)
P	static pressure	eqn. (2.2.2)
P_B	line pressure	sec. (4.3.3)
P_C	static pressure inside the explosion cylinder	eqn. (4.3.1)
$\overline{Pr}$	average Prandtl number of flow through the nozzle	eqn. (4.6.5)
P_ξ	term associated with pressure gradient effect in the general finite-difference equation for ϕ 's	eqn. (B.8)
$(\Delta P)_M$	pressure difference across the mixer	sec. (4.3.3)
$\dot{q}_w''$	rate of heat transfer through the wall of the nozzle passage	eqn. (C.2.1)
Q^r, Q^z	terms expressing the effect of non- uniform density in the finite-difference equation for pressure-correction	eqns.(B.22,B.23)
r	radial co-ordinate	eqn. (2.2.1)
$r_{1/2}$	value of r where the normalised temp- erature is half that at the jet axis	sec. (3.5.4)

<u>Symbols</u>	<u>Meaning</u>	<u>Equation of first mention</u>
r_W	jet-width	sec. (5.2.1)
R	universal gas constant	eqn. (2.3.16)
Re	Reynolds number	sec. (3.5.3)
$\overline{Re}$	average Reynolds number of flow through the nozzle	sec. (4.4.6)
s	order of the polynomials	eqns. (4.6.5-6)
S	source term in the governing differential equation for ϕ 's	sec. (2.6)
t	time co-ordinate	eqn. (2.2.1)
Δt	size of forward-marching time-step	eqn. (3.6.1)
$(\Delta t)_{\max}$	maximum value of Δt	eqn. (3.6.2)
T	temperature	eqn. (2.2.6)
T_b	bulk temperature	eqn. (C.2.2)
$T_{0,I}$	actual temperature of the gas at the nozzle exit	eqn. (4.6.1)
T_f	flame temperature	eqn. (4.6.5)
T^r, T^z	terms associated with diffusion in the general finite-difference equation for ϕ 's	eqns. (B.6, B.7)
U	coefficient in the general finite differ- ence equation for ϕ 's	eqn. (B.10)
v	velocity in radial direction	eqn. (2.2.1)
v_τ	frictional velocity	eqn. (2.3.19)
$\vec{v}$	velocity vector	eqn. (2.3.2)
V_G	volume of the explosion cylinder	eqn. (4.3.3)
v', v'_θ	fluctuating components of radial and circumferential velocities	sec. (2.2)

<u>Symbols</u>	<u>Meaning</u>	<u>Equation of first mention</u>
W	velocity in longitudinal direction	eqn. (2.2.1)
w'	fluctuating component of longitudinal velocity	sec. (2.2)
X, Y, Z	constants derived from polynomial curve fitting of the specific heat of the mixture	eqn. (2.3.17)
z	longitudinal co-ordinate	eqn. (2.2.1)
z_f	position of jet-front	
z^+	normalised longitudinal distance from the wall	eqn. (2.3.19)
ϕ	general dependent variable	eqn. (2.6.2)
α	turbulent intensity	sec. (2.5.1)
α_T	heat transfer coefficient for flow around thermocouple	eqn. (4.6.2)
β	compound concentration variable ($m_{O_2} - m_f$)	eqn. (2.2.16)
β_1, β_2	values of β at the nozzle outlet and in the surroundings	eqn. (2.2.20)
ϵ	dissipation rate of turbulent kinetic energy	sec. (2.3.2)
γ	compound concentration variable ($m_{CO_2} + m_f$)	eqn. (2.2.17)
γ_1, γ_2	values of γ at the nozzle outlet and in the surroundings	eqn. (2.2.20)
Γ_ϕ	diffusivity for property ϕ	eqn. (2.2.4)

<u>Symbols</u>	<u>Meaning</u>	<u>Equation of first mention</u>
κ	pre-exponential constant in Arrhenius expression	eqn. (2.4.1)
θ	time-constant of thermocouple	eqn. (4.6.1)
λ	length scale constant	eqn. (2.5.4)
μ	viscosity	eqn. (2.2.4)
η	a normalised variable associated with flow near oscillating flat plate	eqn. (3.5.1)
ρ	mass-density	eqn. (2.2.1)
δ_ϕ	Schmidts number for variable ϕ	eqn. (2.2.4)
w	equivalence ratio	sec. (2.4.2)
Ω	equivalence ratio 'correction function for Arrhenius expression	eqn. (2.4.1)
τ	shear stress	eqn. (2.2.2)
τ_s	wall shear stress	sec. (2.3.5)
ξ	a normalised variable in the study of impulsively-starting jet	sec. (3.5.3)
ψ	polytropic constant	eqn. (4.3.1)

Subscripts

0	along the jet axis
1	in longitudinal direction
2	in radial direction
3	in circumferential direction
atm	atmospheric condition

A	denotes Arrhenius 'global' model
b	fully-burnt condition
c	condition inside the explosion cylinder
CO ₂	denotes carbon-dioxide
D	at the present time-step
e,w,n,s	at points mid-way between P and E,W,N,S
E,W,N,S	at points east, west, north and south of point P
eff	effective value of the quantity concerned
f	denotes fuel
G	in the surroundings
H	pertaining to total stagnation enthalpy
H ₂ O	denotes steam
i	initial condition
I	at the nozzle exit
ISEN	values of variables obtained by assuming isentropic flow
j	denotes species j
jet	values of variables obtained by assuming impulsively-starting condition
k	pertaining to turbulent kinetic energy
N ₂	denotes nitrogen
O ₂	denotes oxygen
P	at the point under investigation
ref	values of variables evaluated at reference condition
t	turbulent value of the quantity concerned
T	denotes thermocouple
u	denotes unburnt-condition
U	at the previous time-step

β	pertaining to the compound concentration variable β
γ	pertaining to the compound concentration variable γ
$\emptyset$	pertaining to property $\emptyset$

Superscripts

*	denotes the estimated value of the quantity concerned
**	denotes a normalised value of the quantity in the impulsively-starting flow investigation
'	denotes the correction of the quantity concerned
—	with the upwind-difference technique being introduced
I	denotes ideal condition
P	pertaining to static pressure
r	in the radial direction
t	value of the variable at the present time-step
t-1	value of the variable at the previous time-step
V	pertaining to radial velocity
W	pertaining to longitudinal velocity
z	in the longitudinal direction

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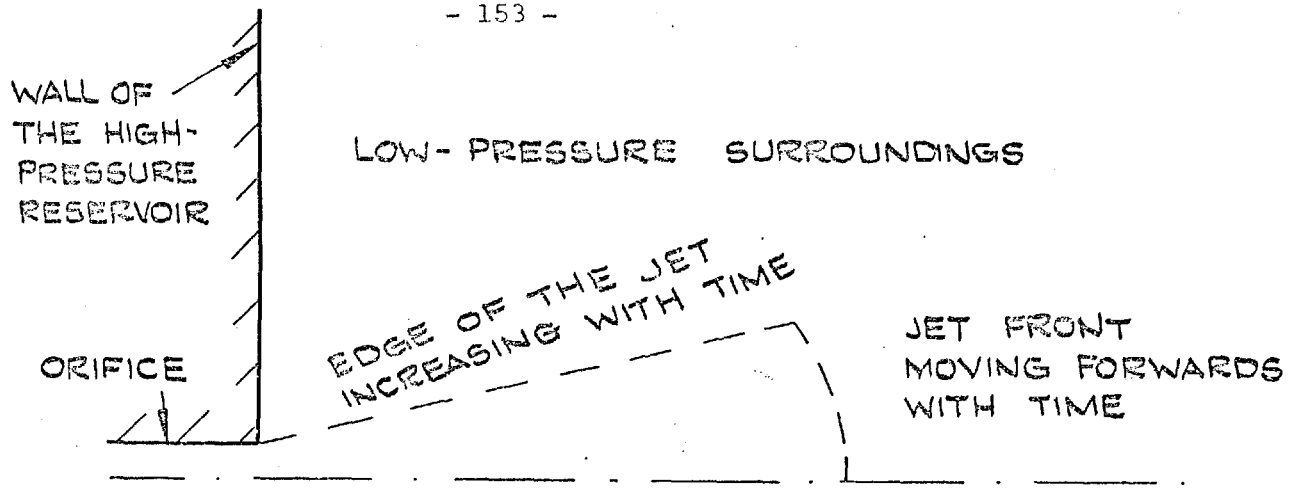


FIG.1.1-1: THE GEOMETRICAL ARRANGEMENT OF THE PHENOMENON CONSIDERED.

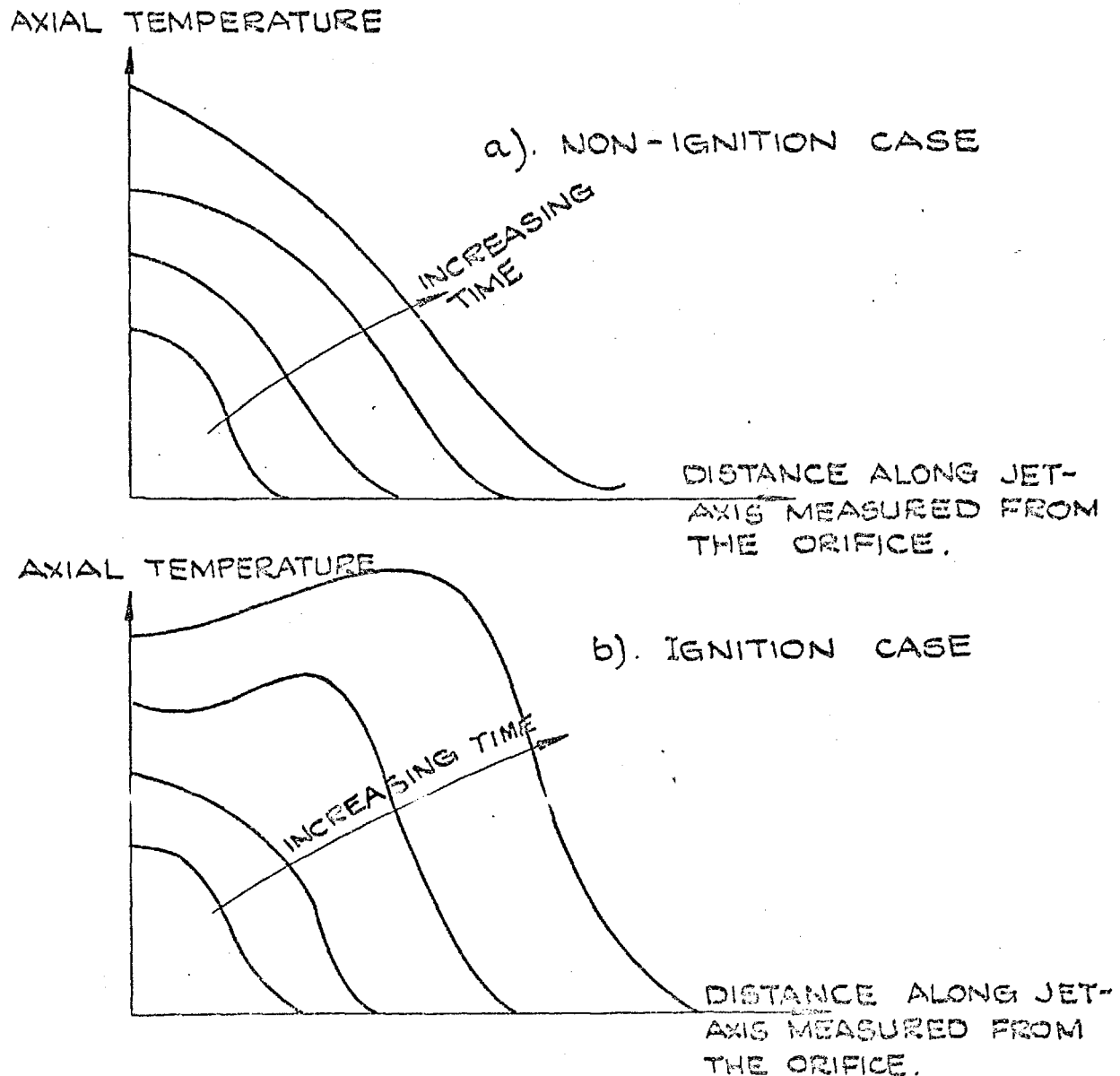


FIG.1.1-2: ESTIMATED DISTRIBUTION AND DEVELOPMENT OF AXIAL TEMPERATURE.

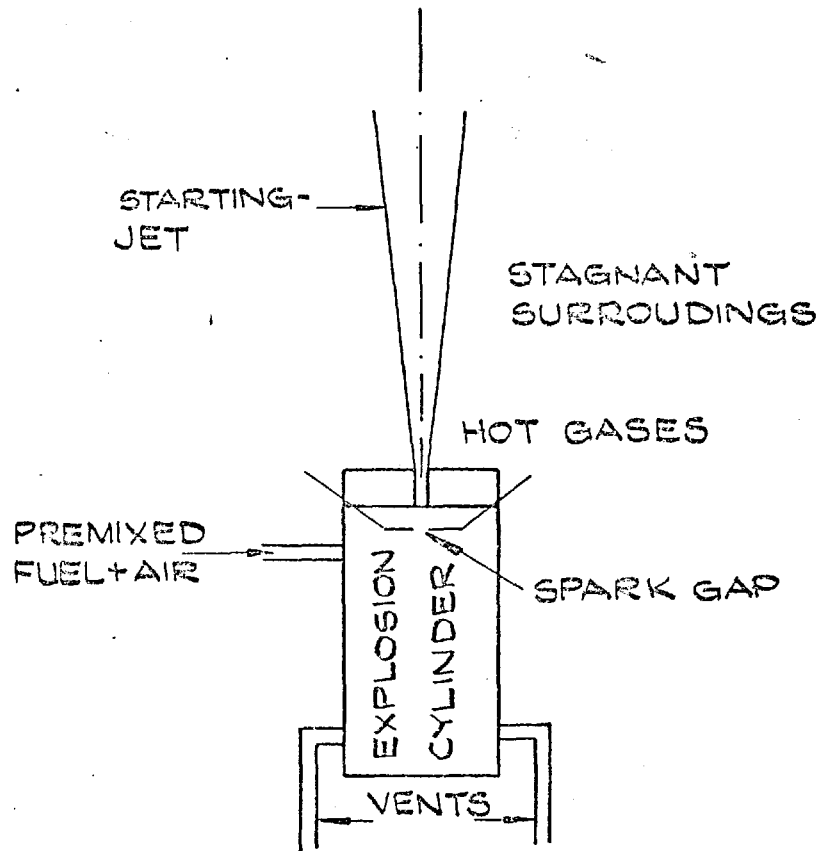


FIG.2.1-1: THE PHYSICAL ARRANGEMENT OF THE PROBLEM.

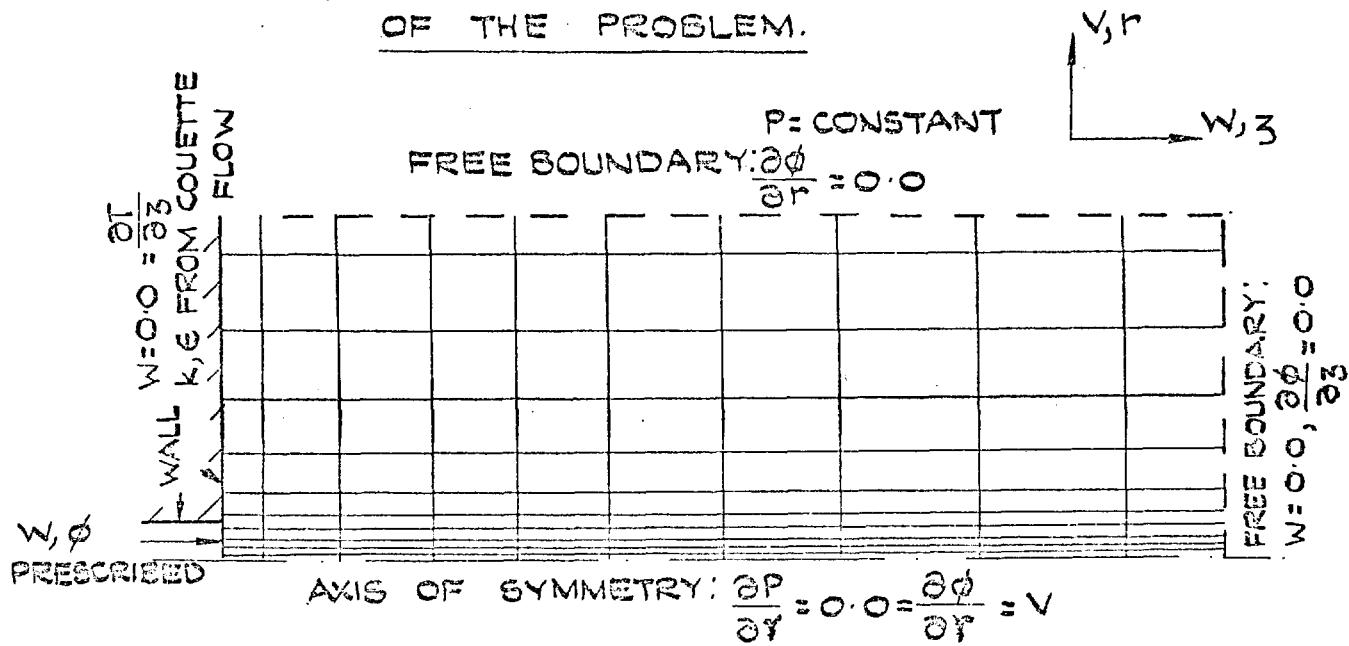


FIG.2.6-1: THE FLOW DOMAIN AND BOUNDARY CONDITIONS.

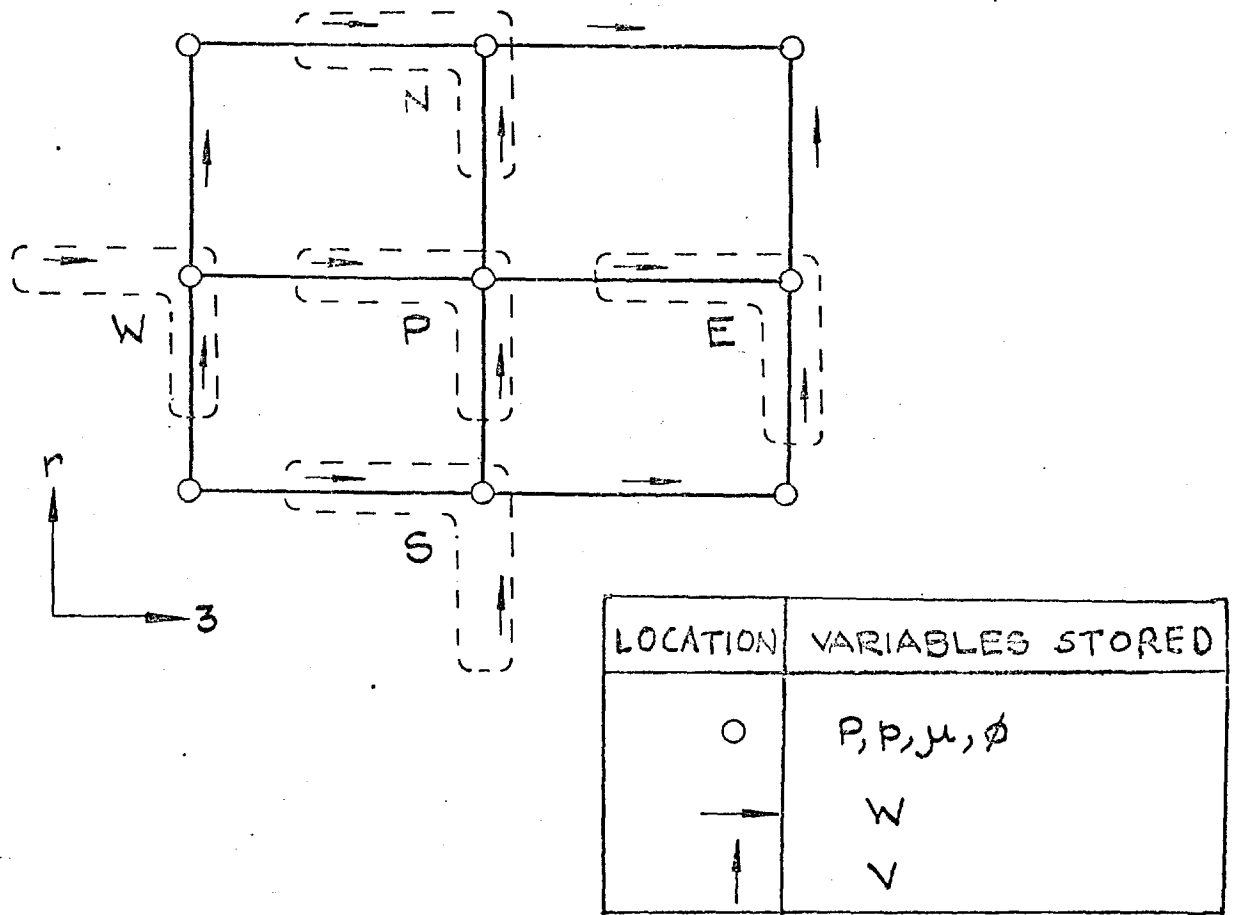


FIG. 3.2-1: THE STAGGERED GRID

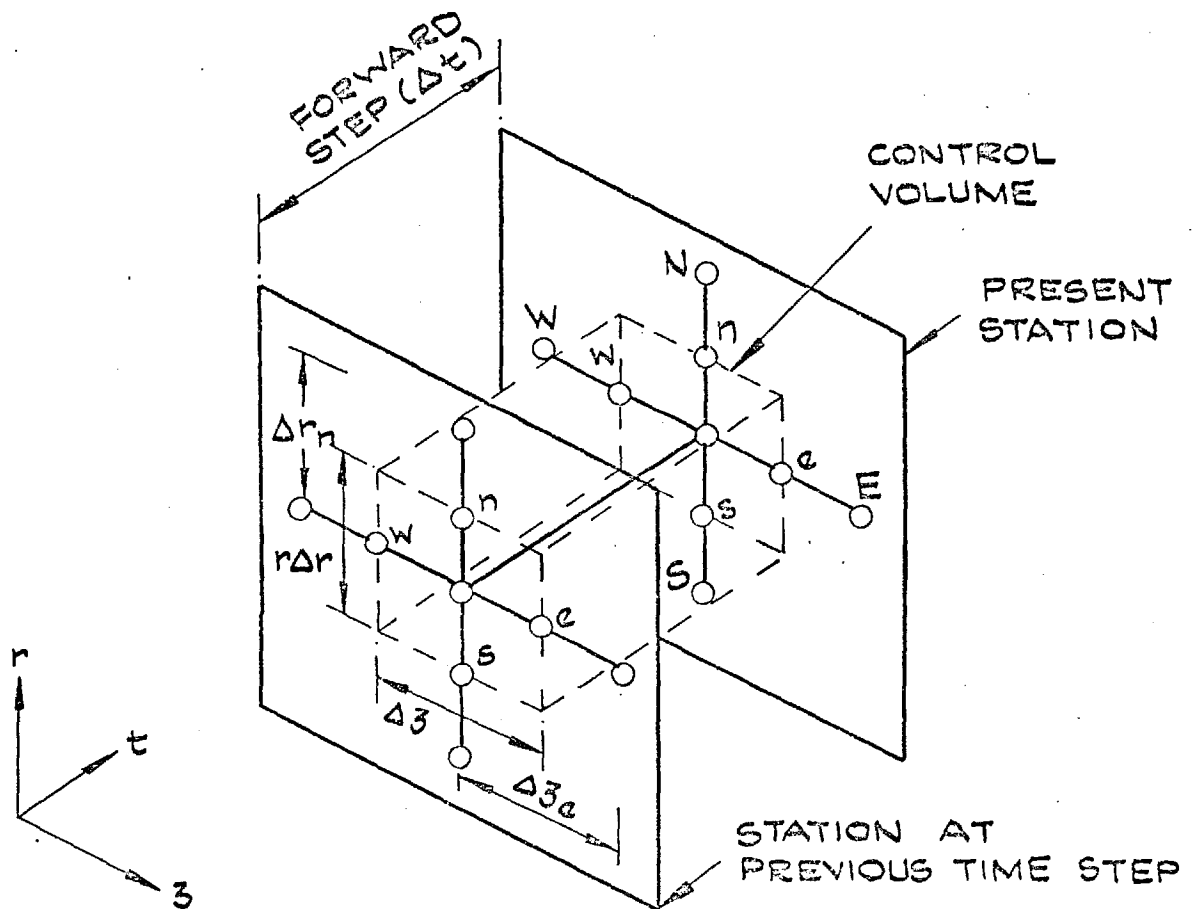


FIG. 3.2-2: THE FINITE - DIFFERENCE CONTROL VOLUME.

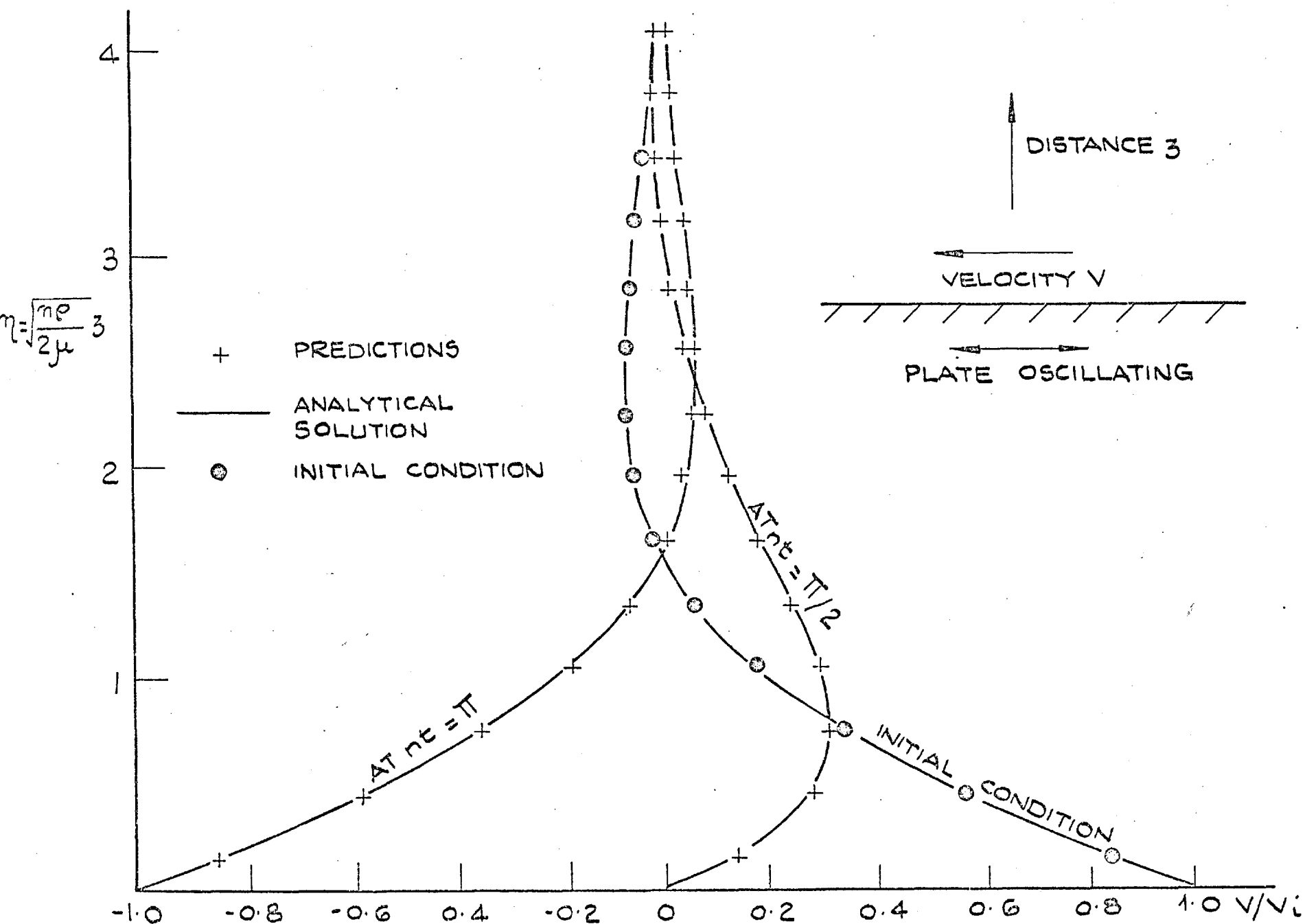


FIG.35-VELOCITY PROFILES NEAR AN OSCILLATING FLAT PLATE.

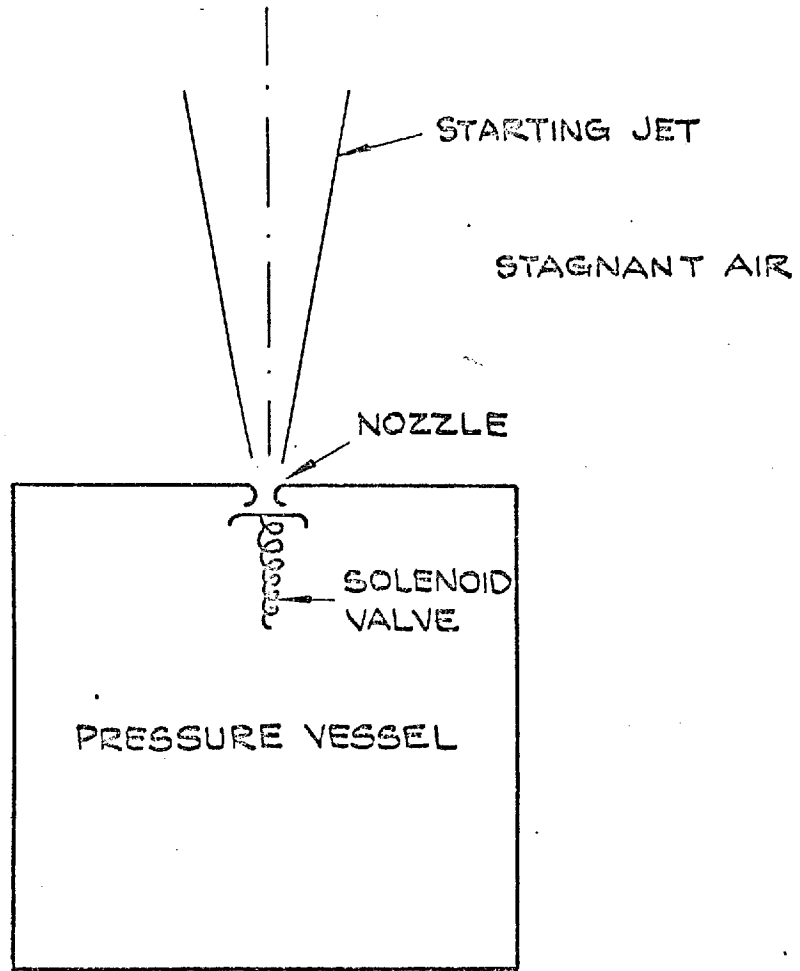


FIG. 3.5-2: THE STARTING-JET FLOW
CONSIDERED BY MA & ONG (1971).

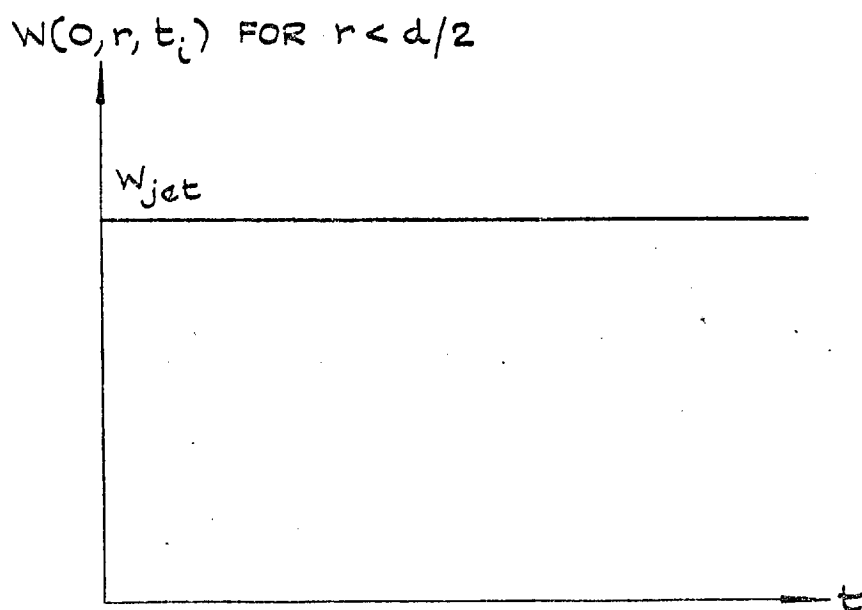


FIG. 3.5-3: THE IMPULSIVELY-STARTING CONDITION.

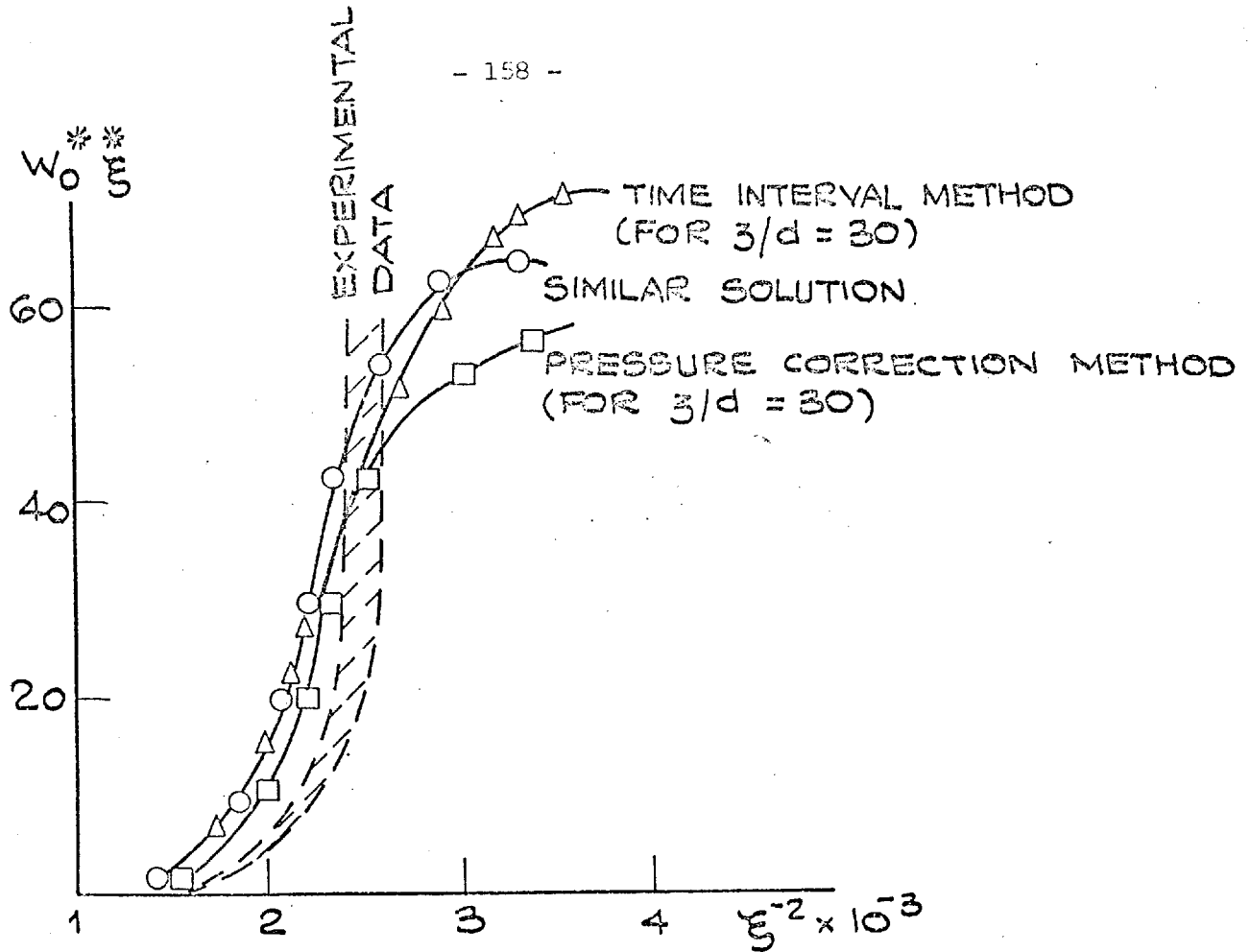


FIG. 3.5-4: COMPARISON OF PREDICTIONS (CONSTANT μ_{eff}) WITH EXPERIMENTAL RESULTS.

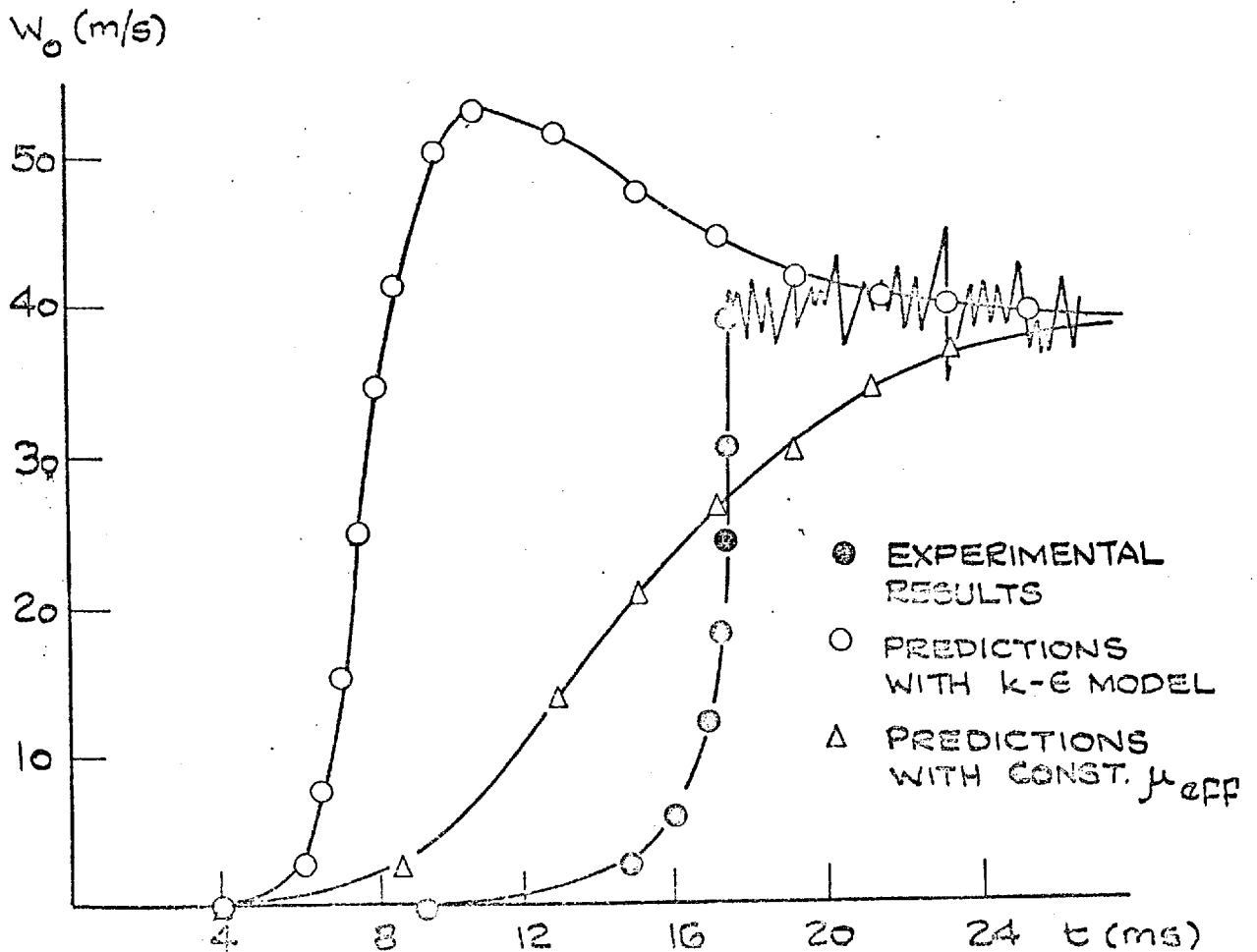


FIG. 3.5-5: AXIAL VELOCITY DEVELOPMENT FOR 1" DIAMETER NOZZLE AT $3/d = 20$

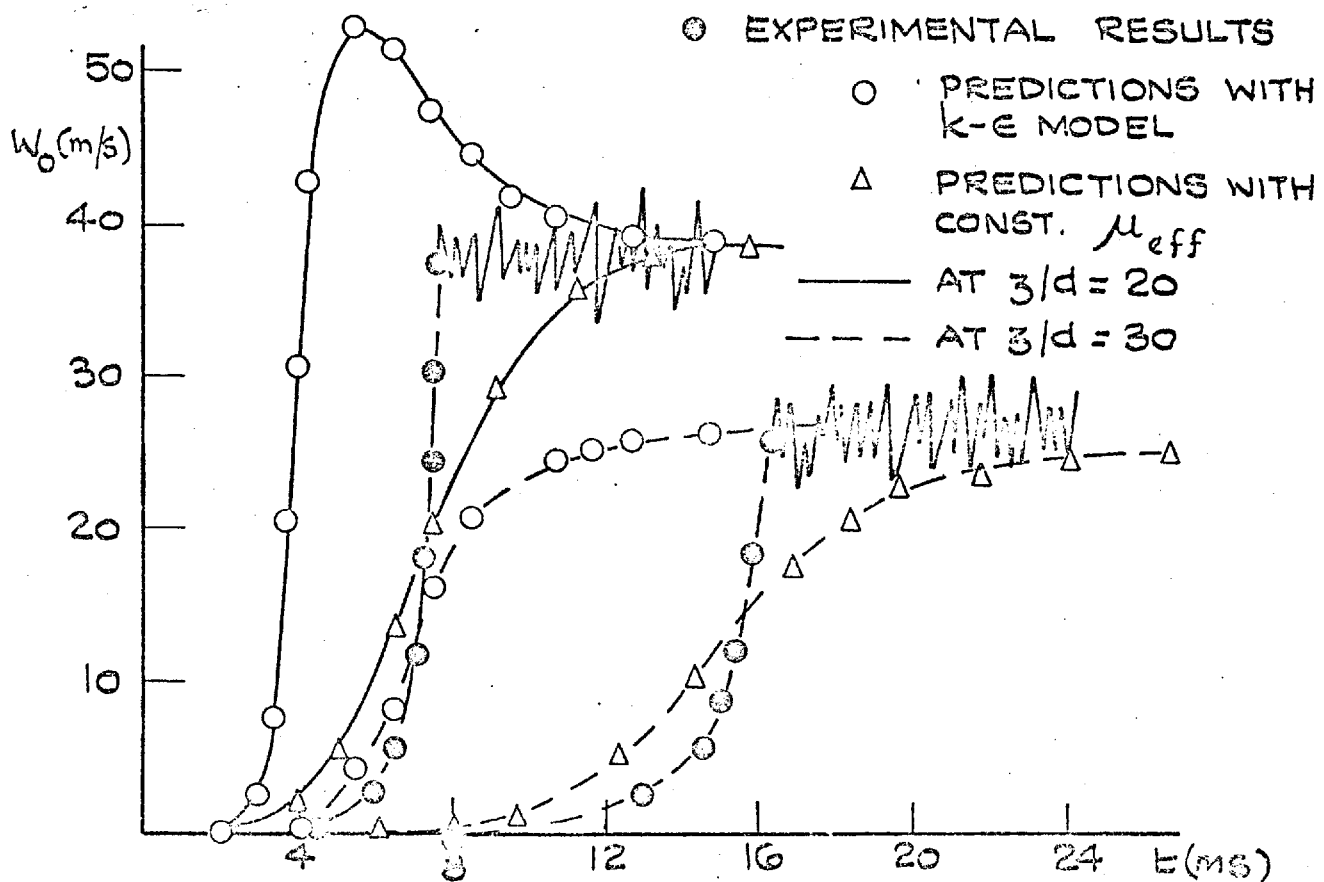
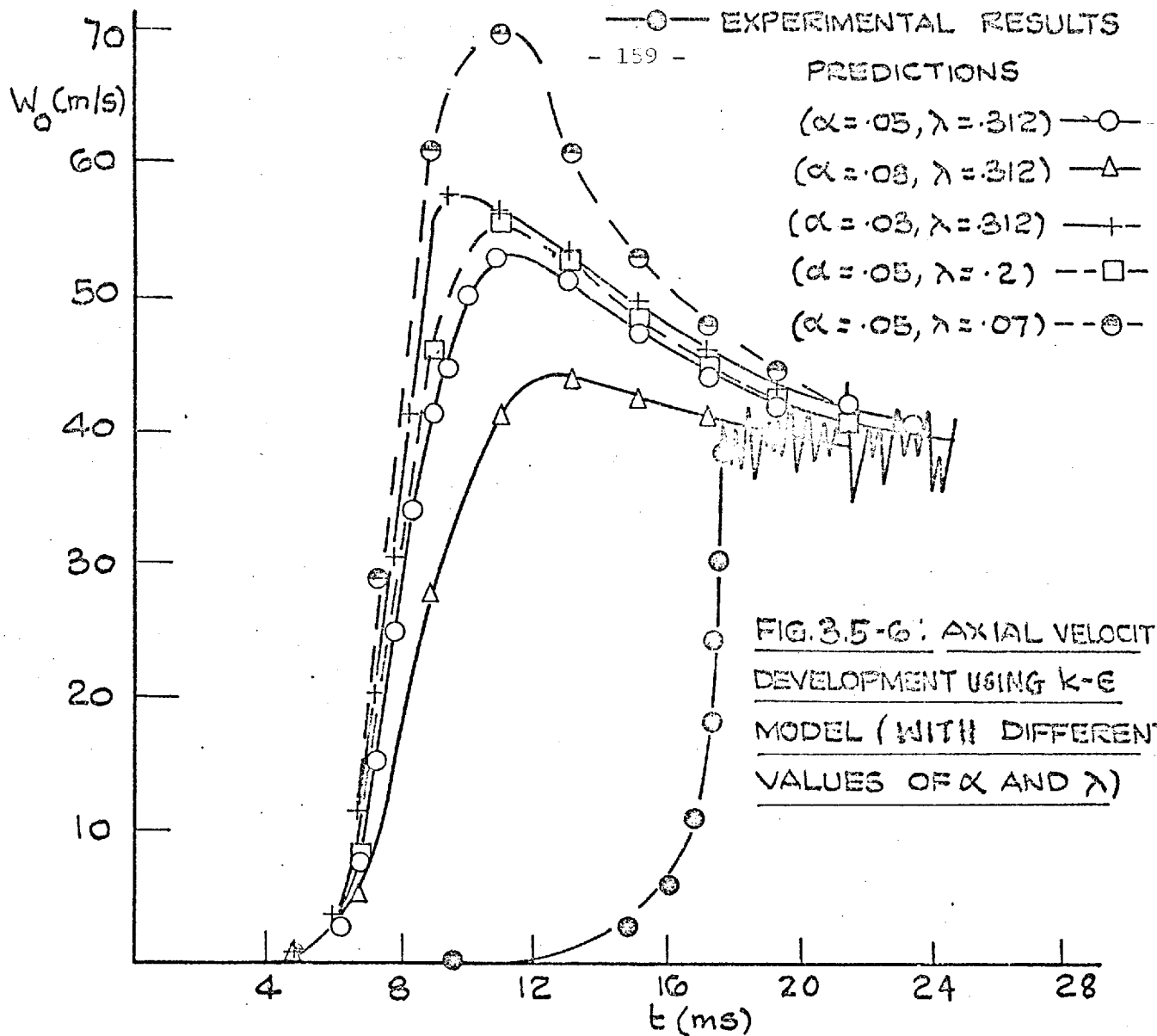


FIG. 3.5-7: AXIAL VELOCITY DEVELOPMENT FOR .5" DIAMETER NOZZLE.

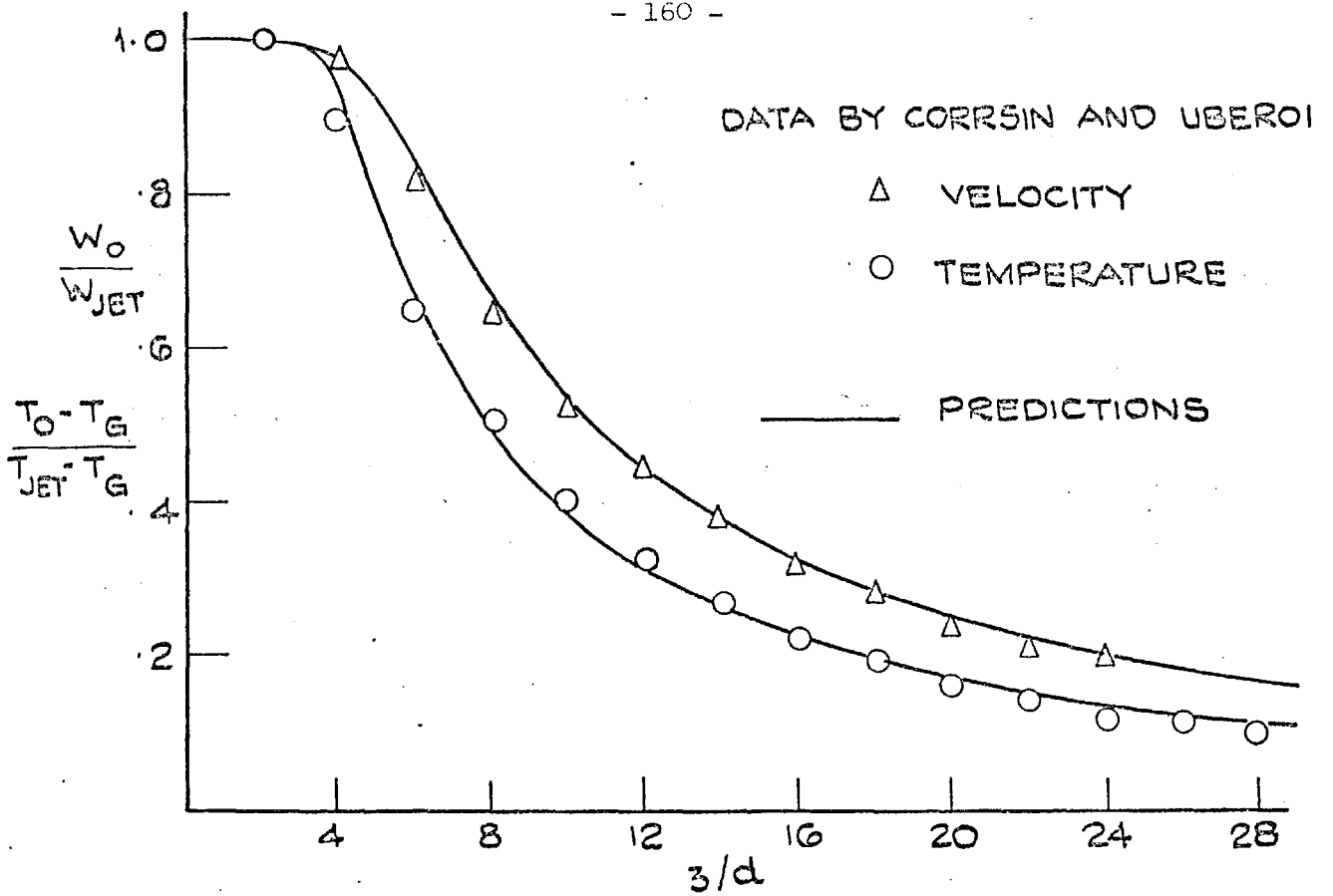


FIG.3.5-8: AXIAL VELOCITY AND TEMPERATURE DISTRIBUTIONS FOR STEADY JET.

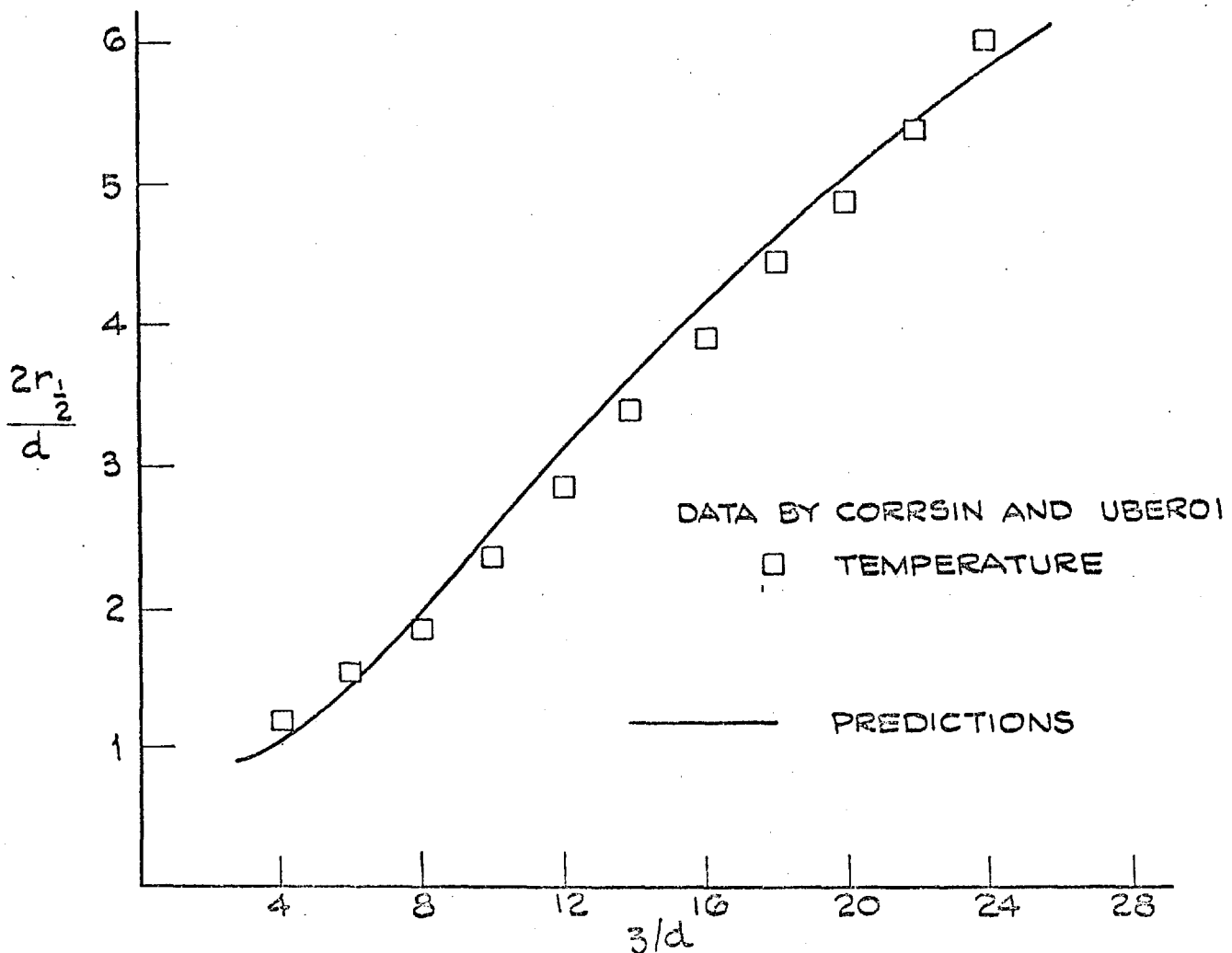


FIG.3.5-9: RADIAL TEMPERATURE DISTRIBUTION FOR STEADY JET.

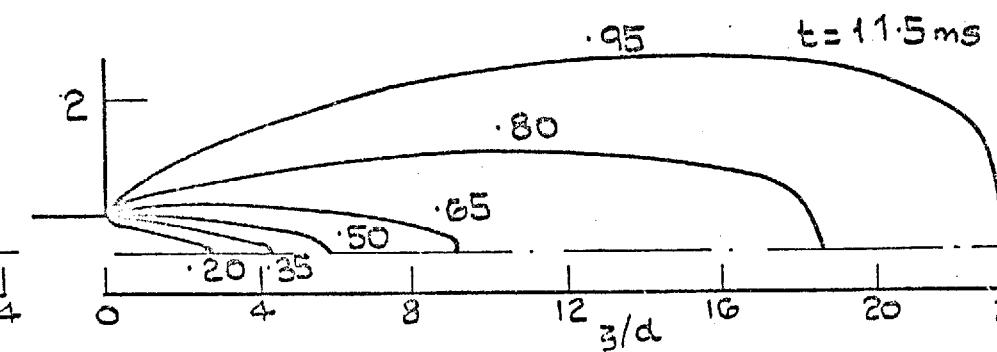
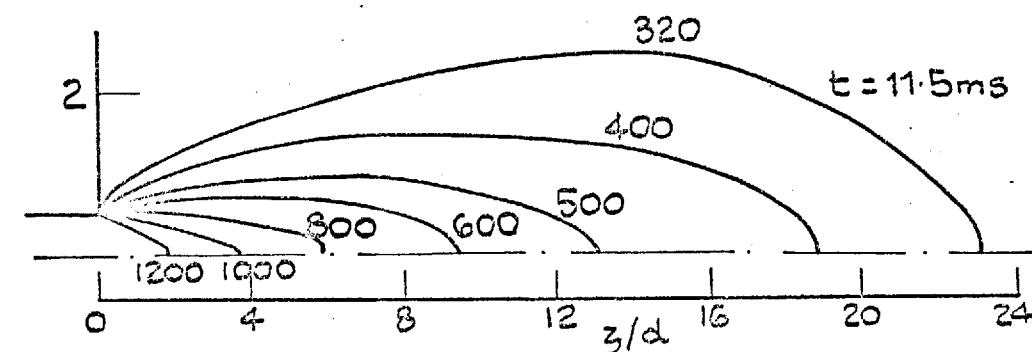
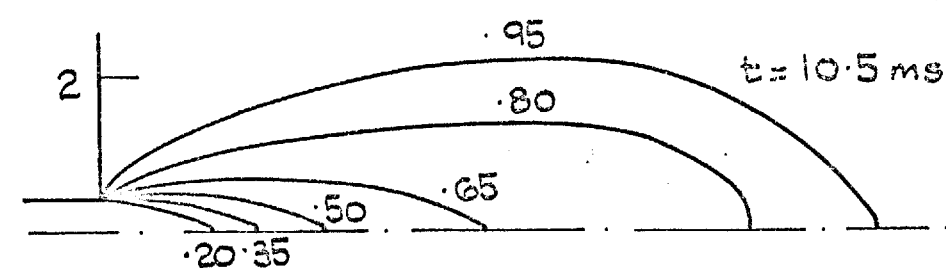
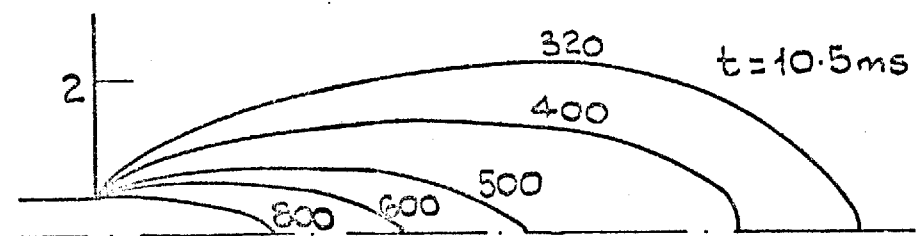
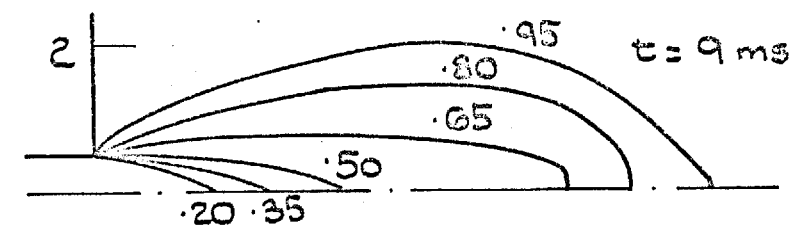
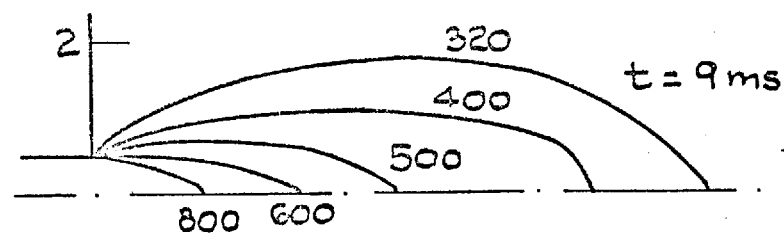
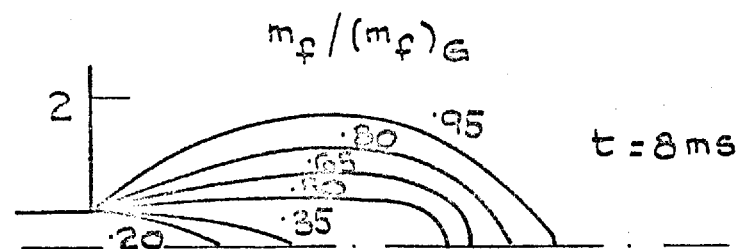
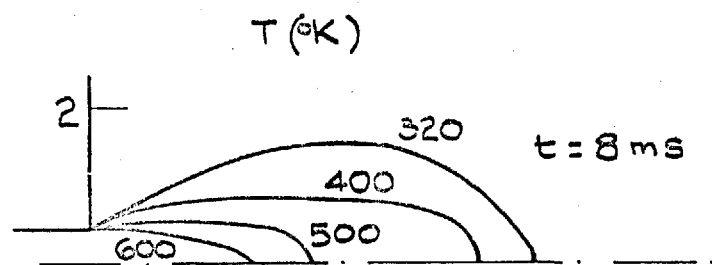


FIG.3.6-1: DISTRIBUTIONS OF TEMPERATURE AND FUEL CONCENTRATION AT FOUR DIFFERENT

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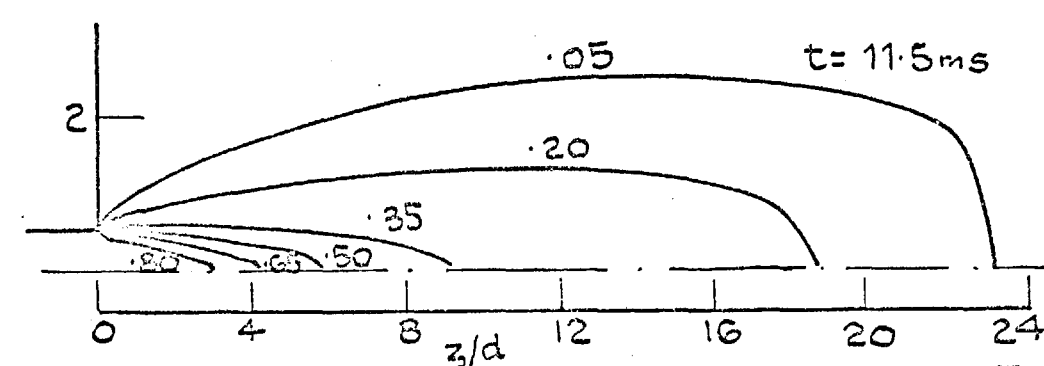
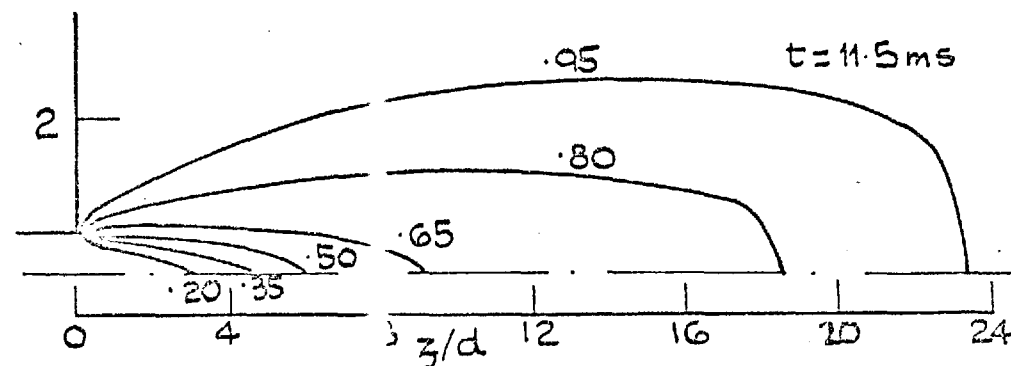
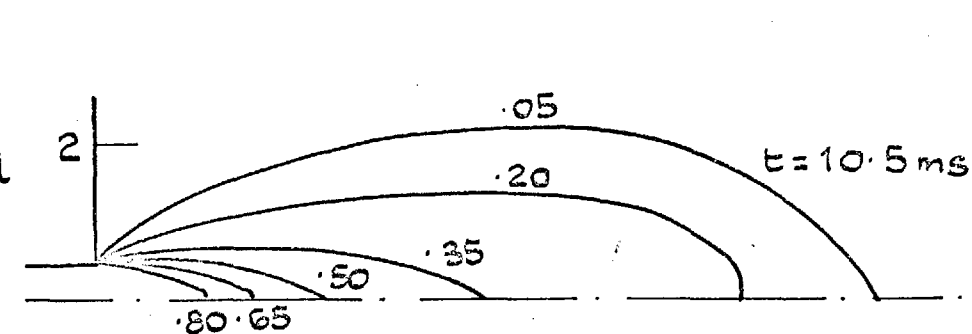
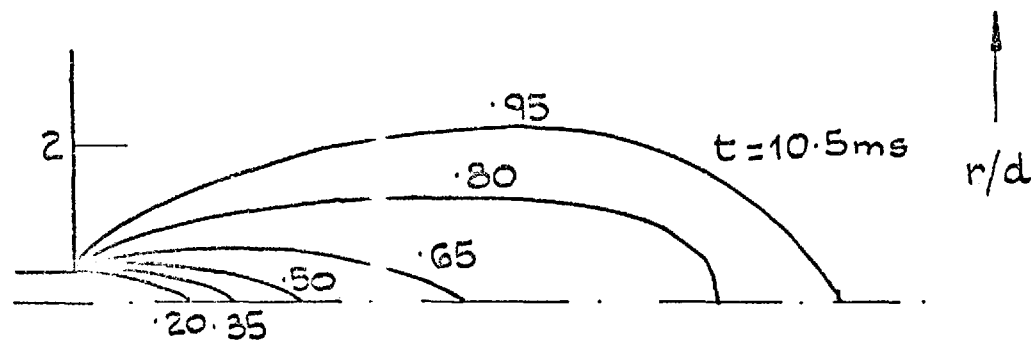
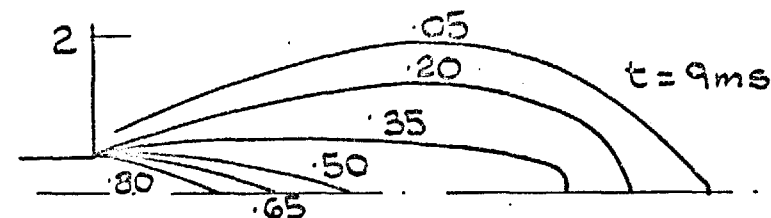
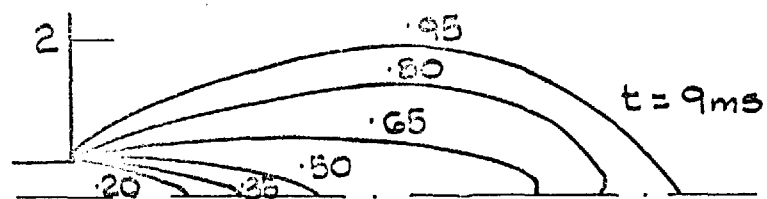
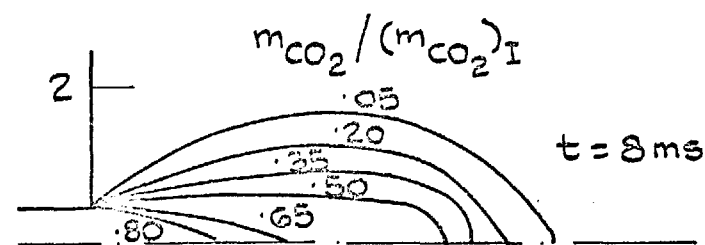
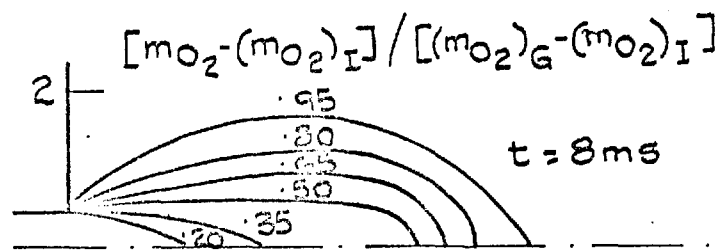


FIG. 3.6-2: DISTRIBUTIONS OF OXYGEN AND CARBONDIOXIDE CONCENTRATIONS AT FOUR DIFFERENT TIME-INTERVALS FOR NON-IGNITION CASE.

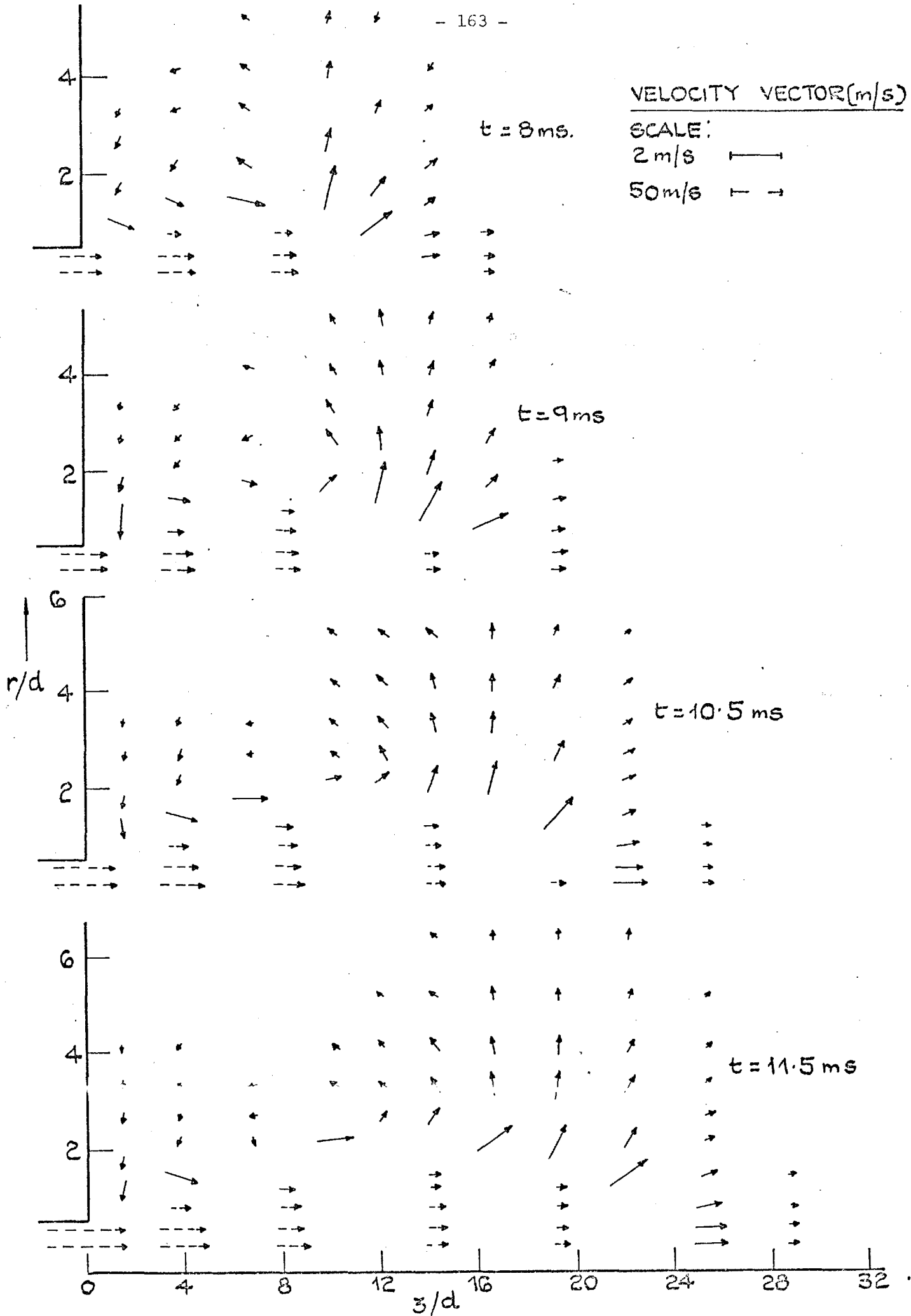


FIG. 3.6-3: VELOCITY-VECTOR DISTRIBUTION AT FOUR DIFFERENT TIME-INTERVALS FOR NON-IGNITION CASE.

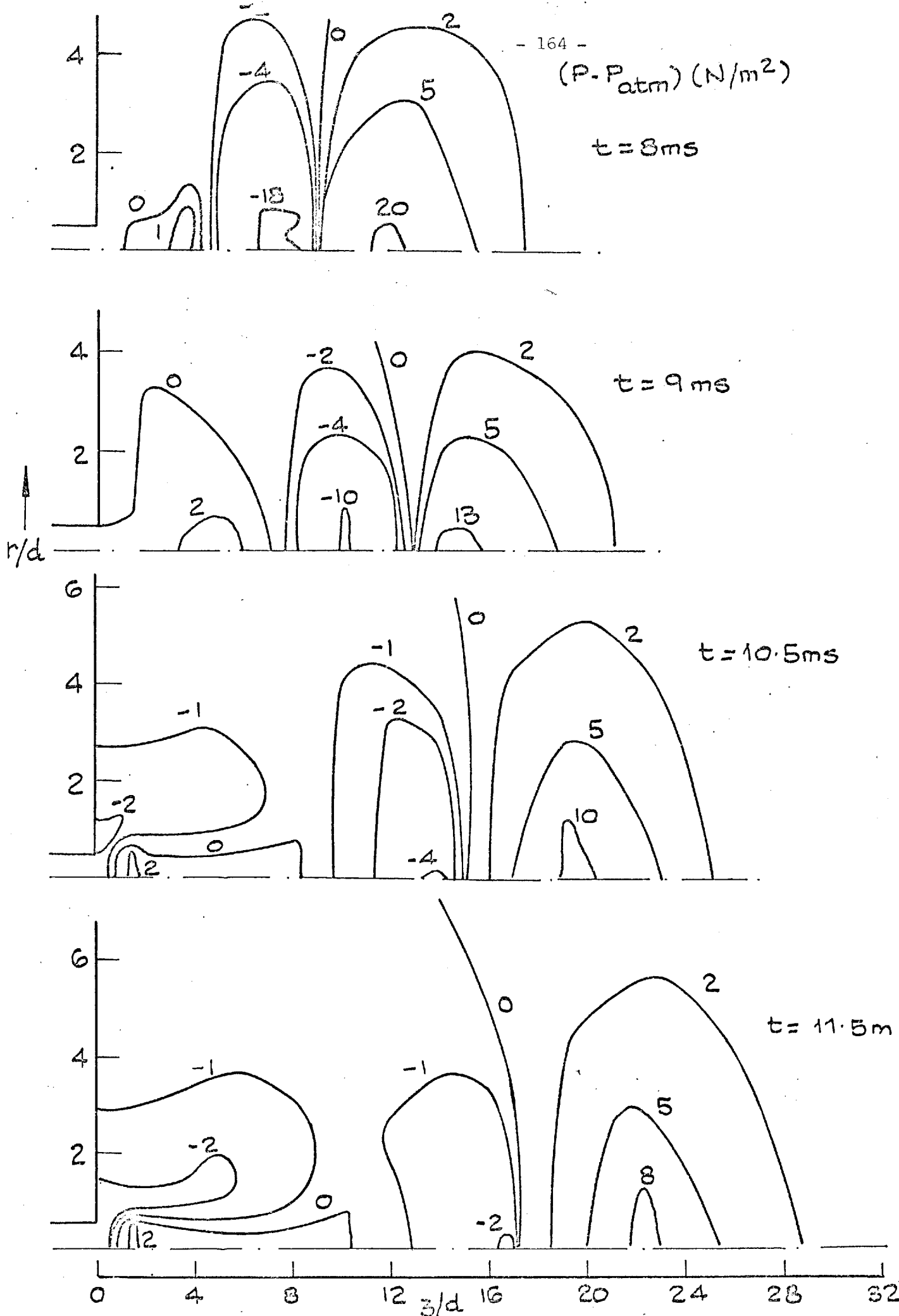


FIG.3.64: STATIC PRESSURE DISTRIBUTION AT FOUR DIFFERENT TIME INTERVALS FOR NON-IGNITION CASE.

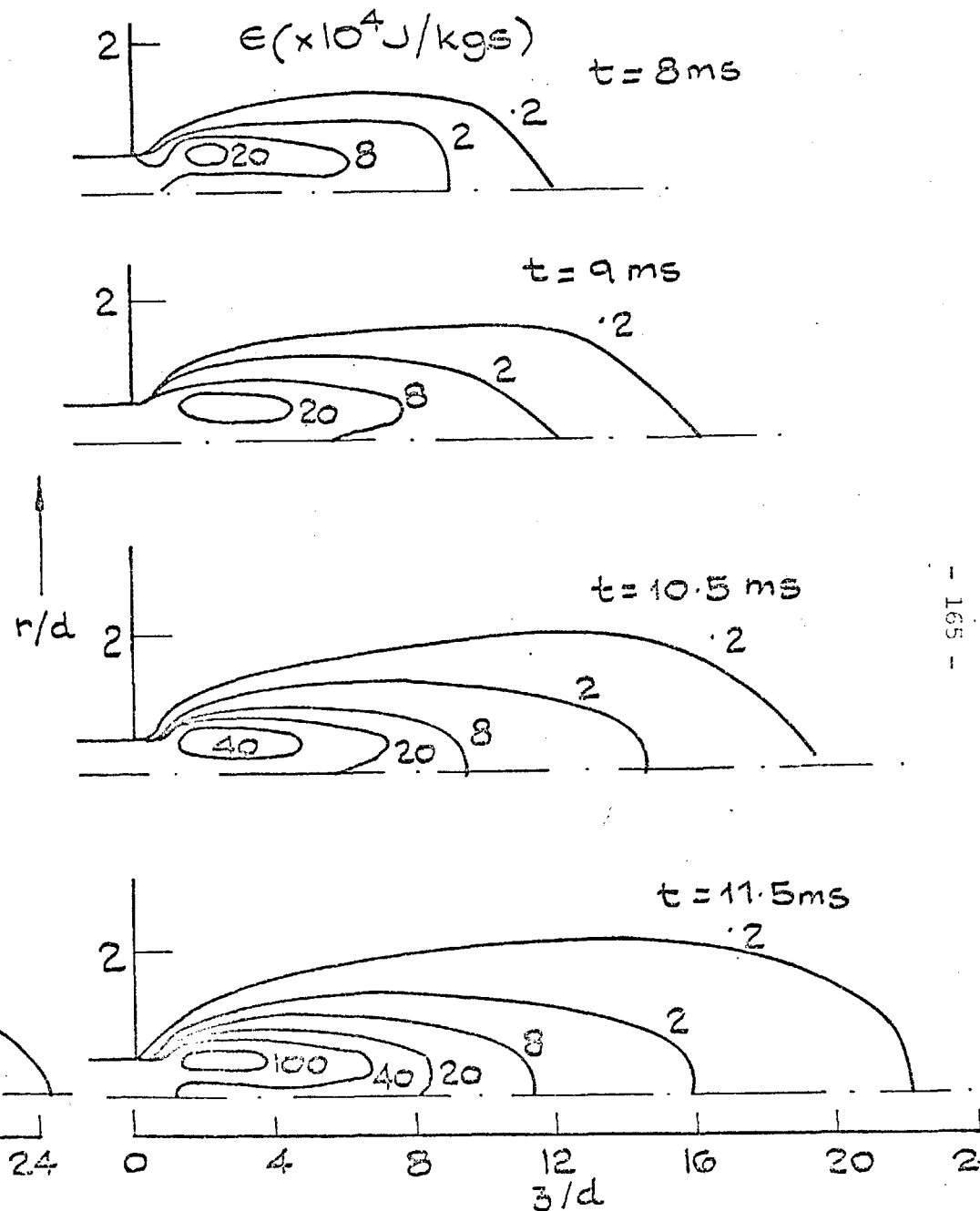
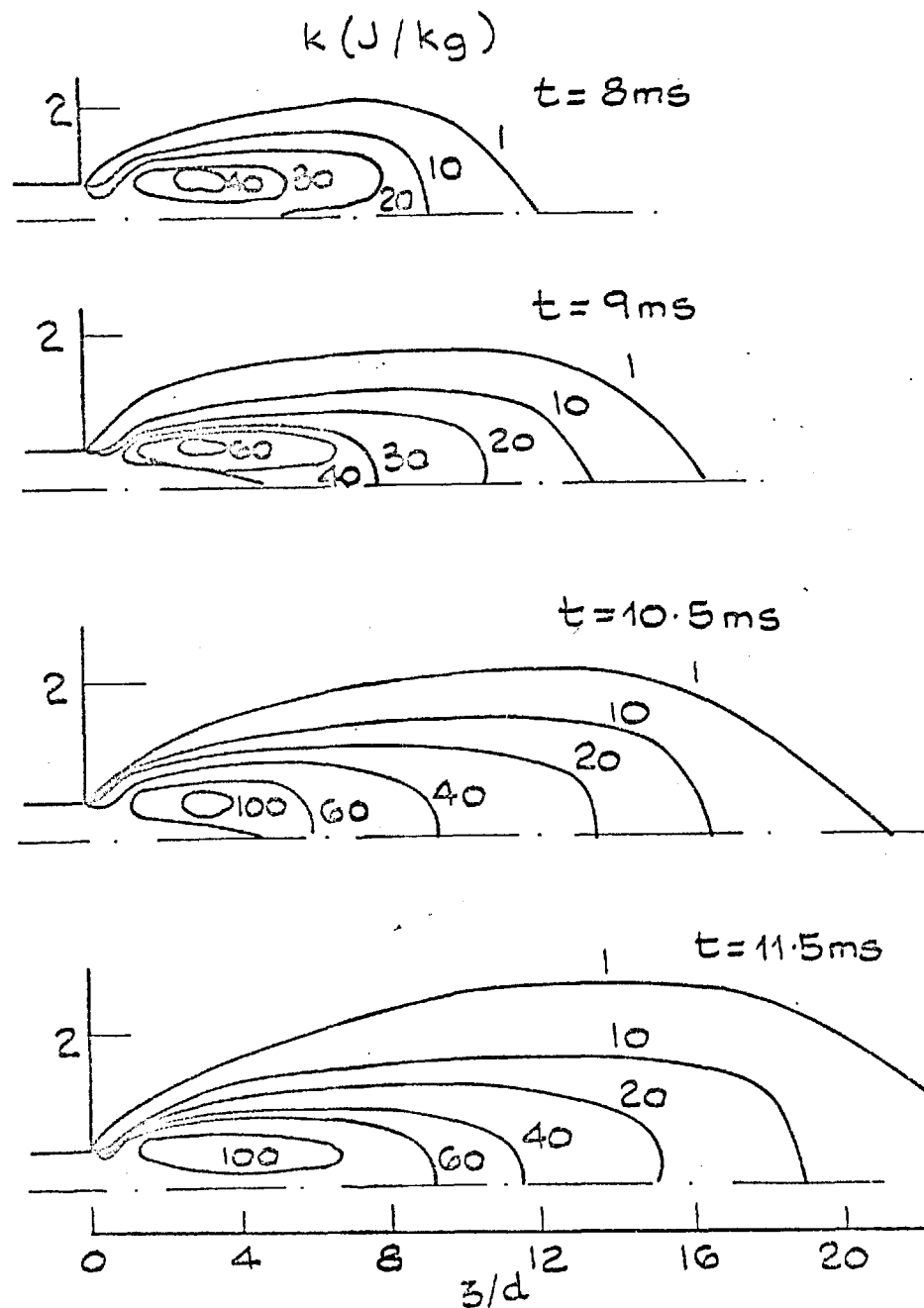


FIG.3.65: DISTRIBUTIONS OF TURBULENT KINETIC ENERGY AND ITS DISSIPATION RATE
 AT FOUR DIFFERENT TIME-INTERVALS FOR NON-IGNITION CASE.

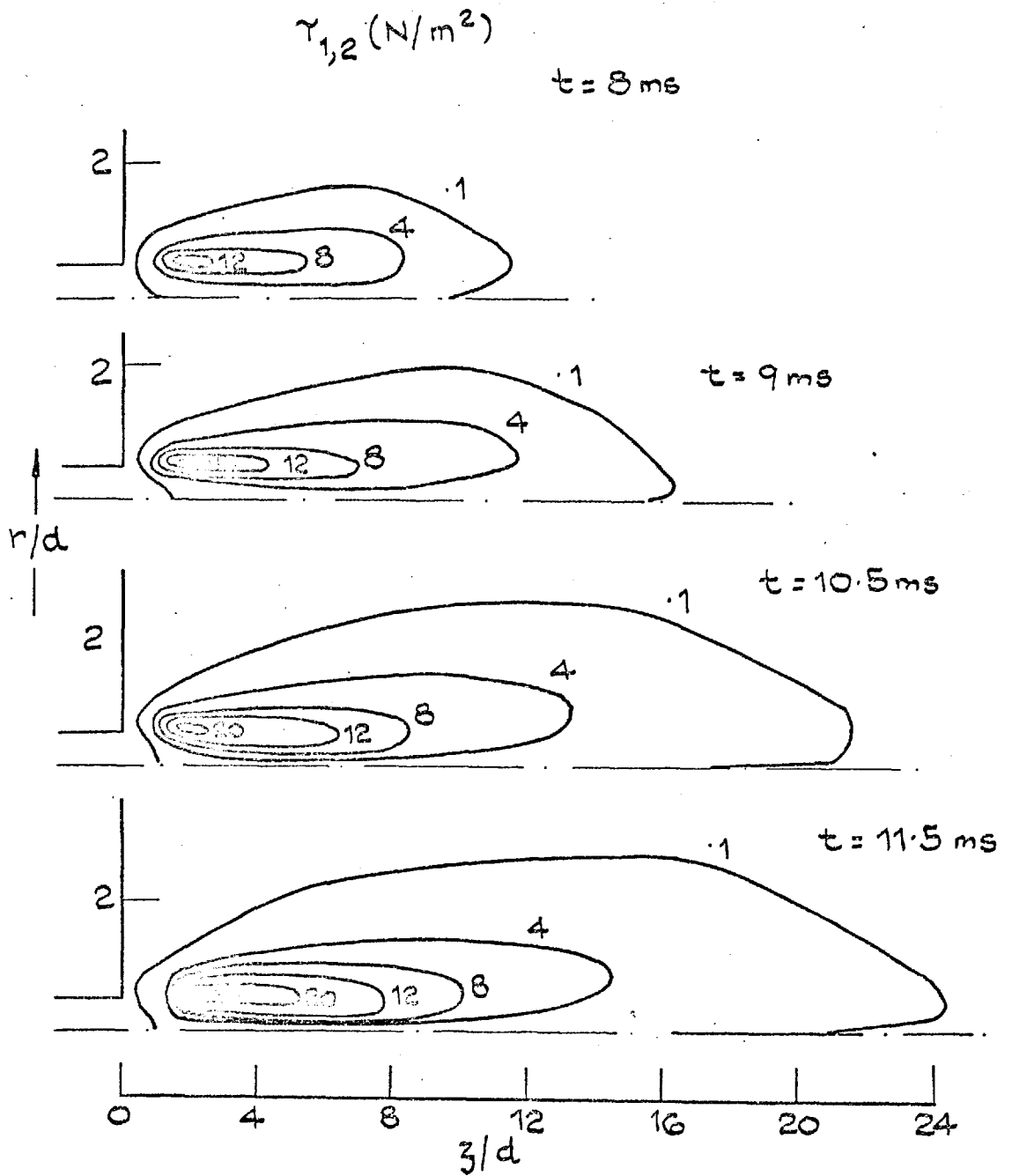


FIG. 3.G-6: DISTRIBUTION OF SHEAR STRESS AT
FOUR DIFFERENT TIME-INTERVALS
FOR NON-IGNITION CASE.

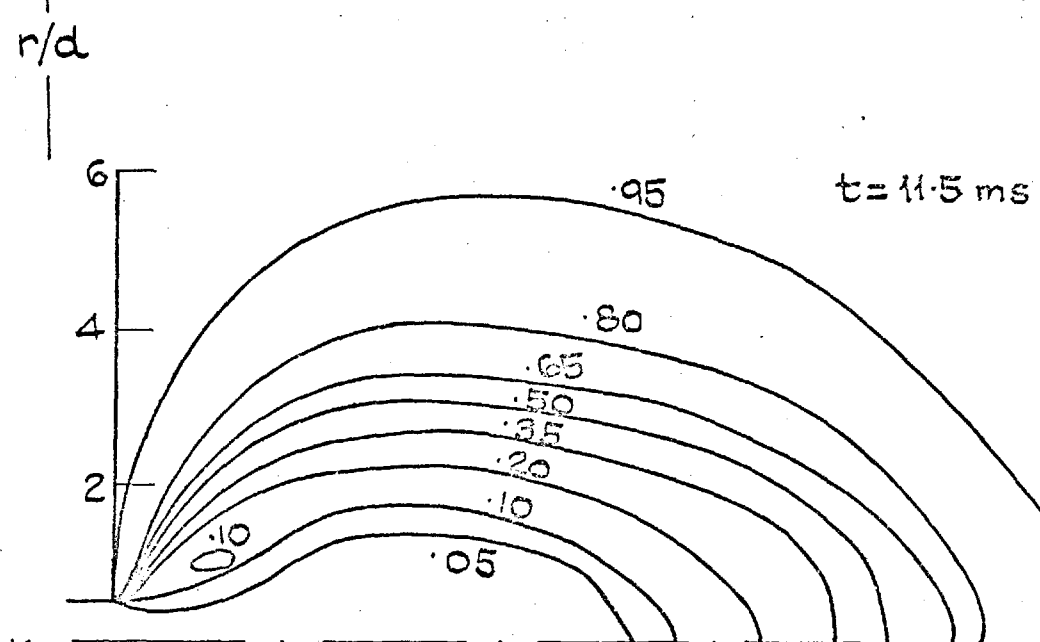
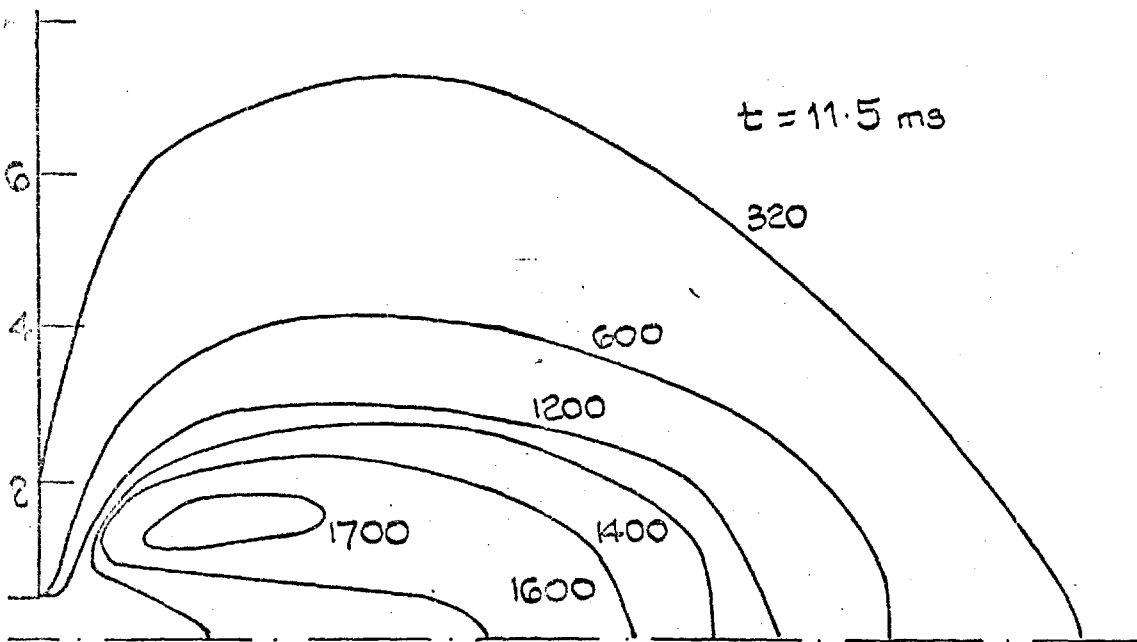
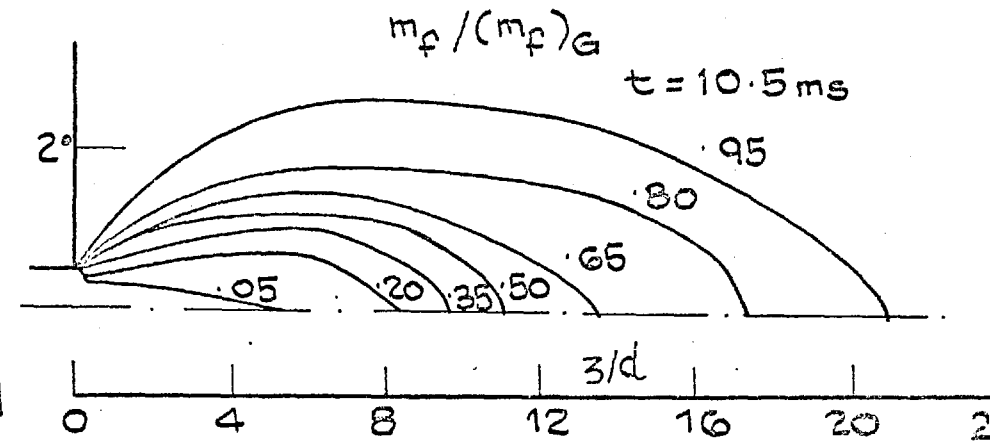
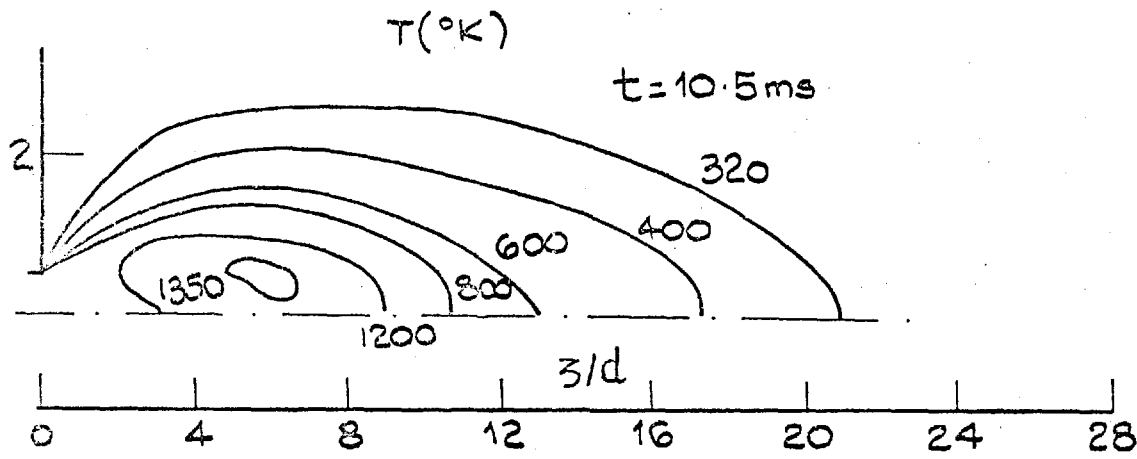


FIG. 3.6-7: DISTRIBUTIONS OF TEMPERATURE AND FUEL CONCENTRATION AT TWO DIFFERENT TIME-INTERVALS FOR IGNITION CASE.

VELOCITY VECTOR (m/s)

SCALE: 10 m/s ———

50 m/s ———

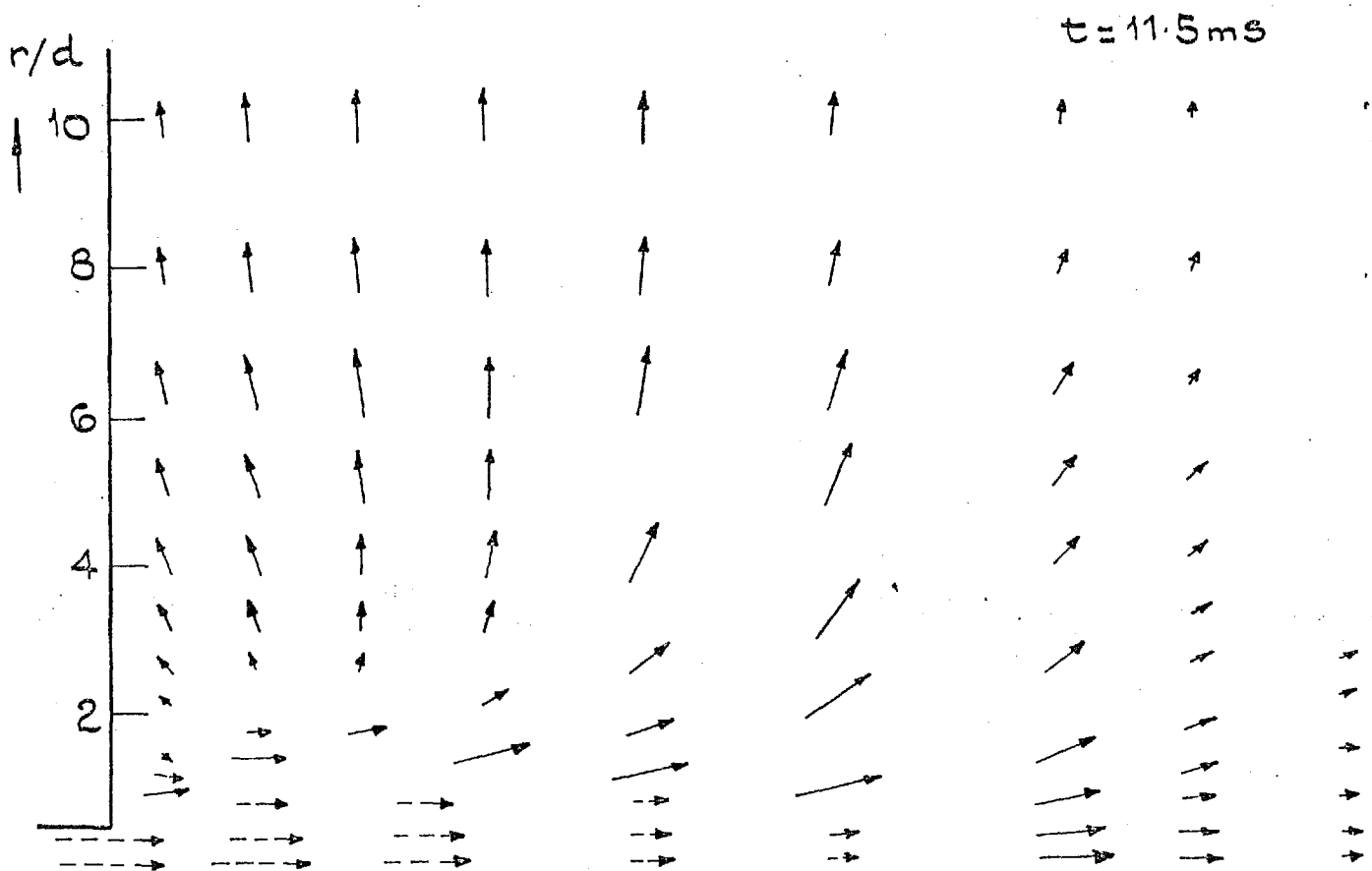
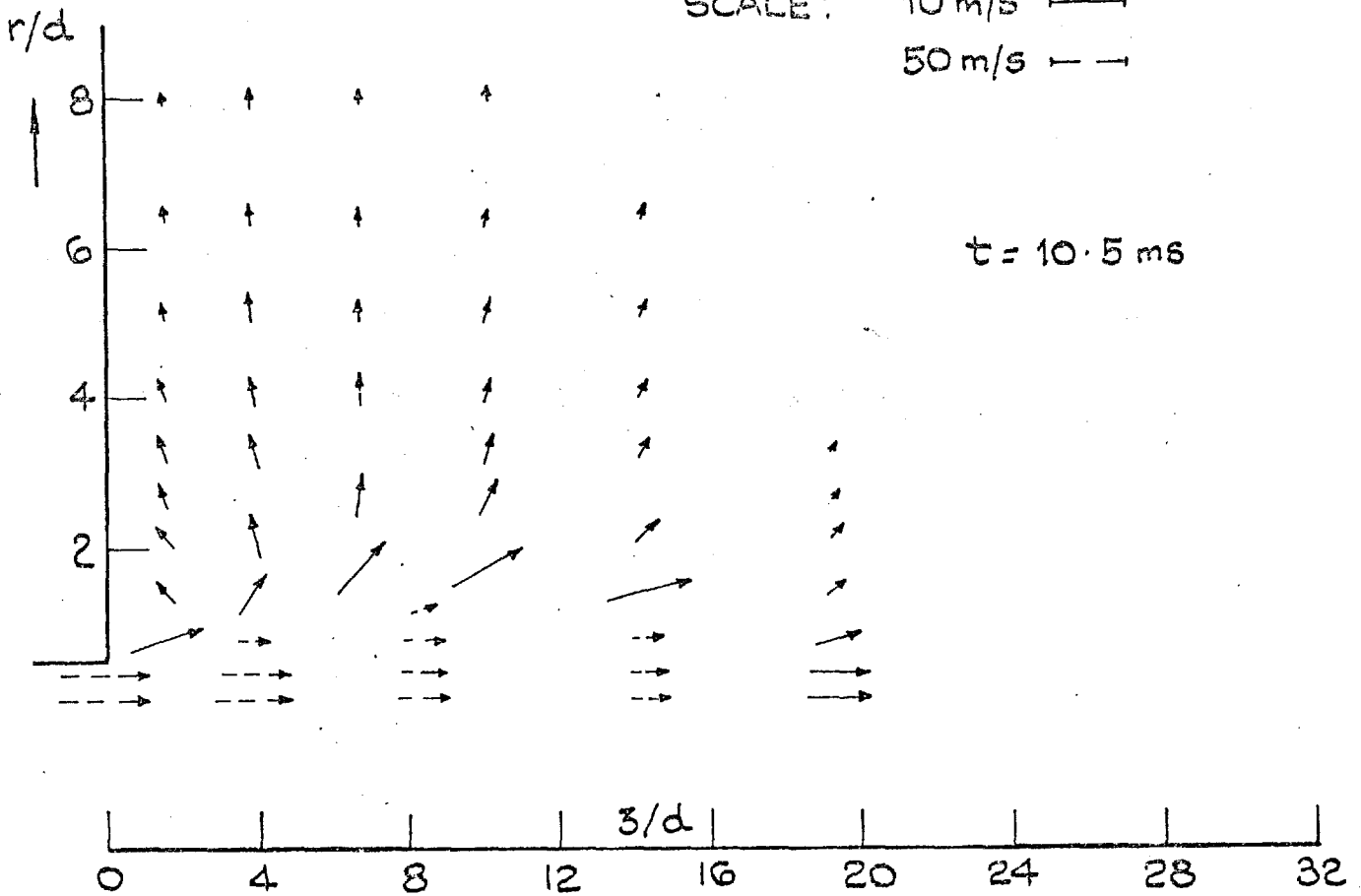


FIG.3.6-8: VELOCITY- VECTOR DISTRIBUTION AT TWO DIFFERENT TIME- INTERVALS FOR IGNITION CASE.

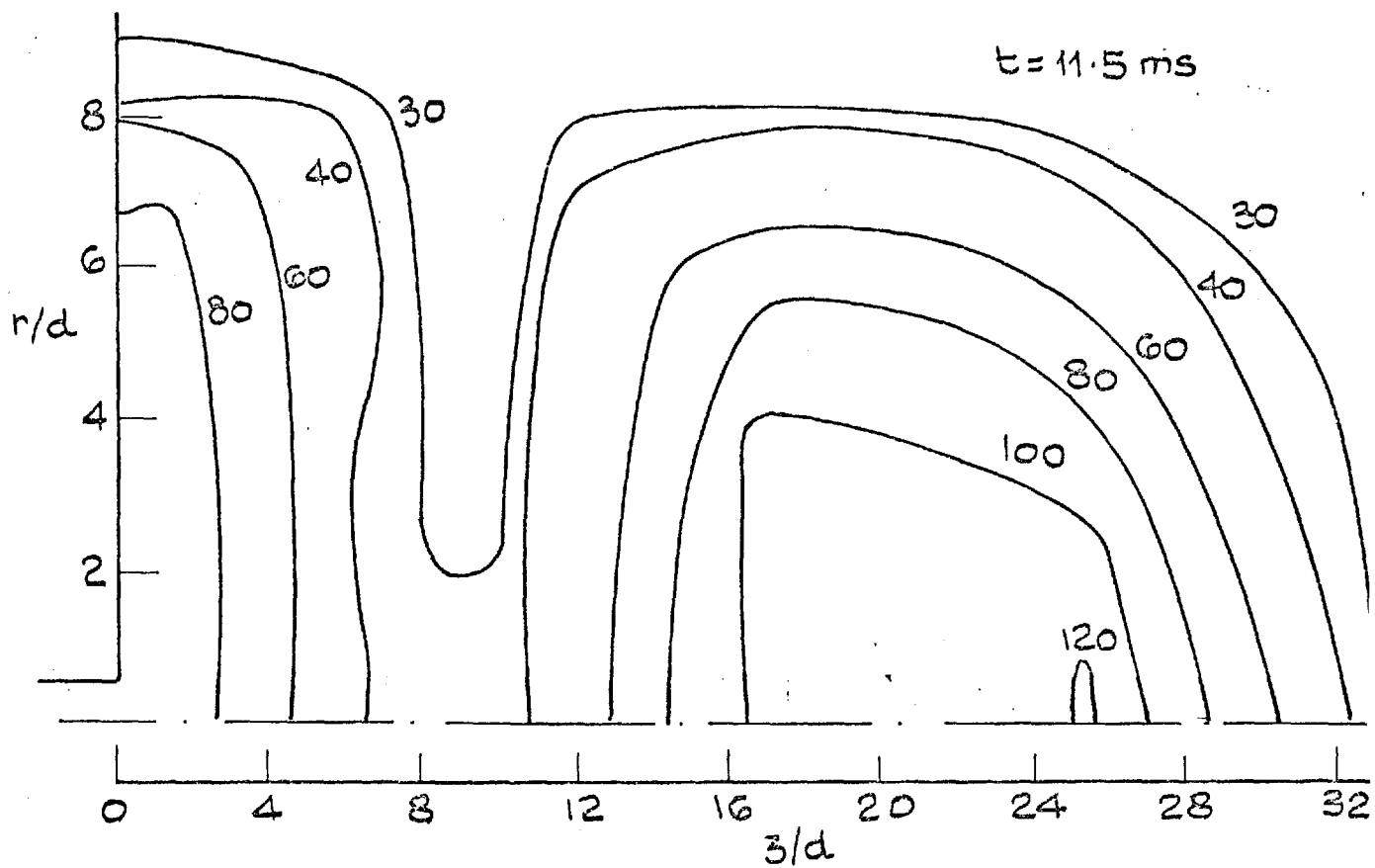
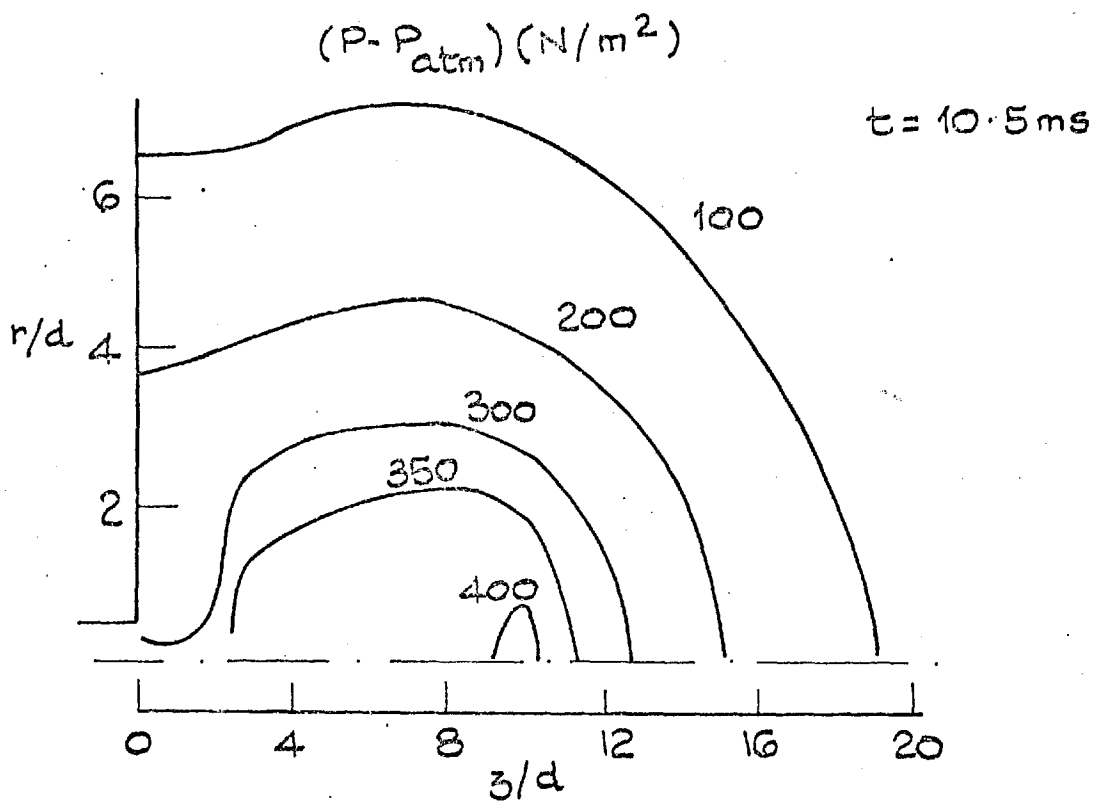


FIG.3.6.9: STATIC PRESSURE DISTRIBUTION AT TWO
DIFFERENT TIME - INTERVALS FOR IGNITION CASE

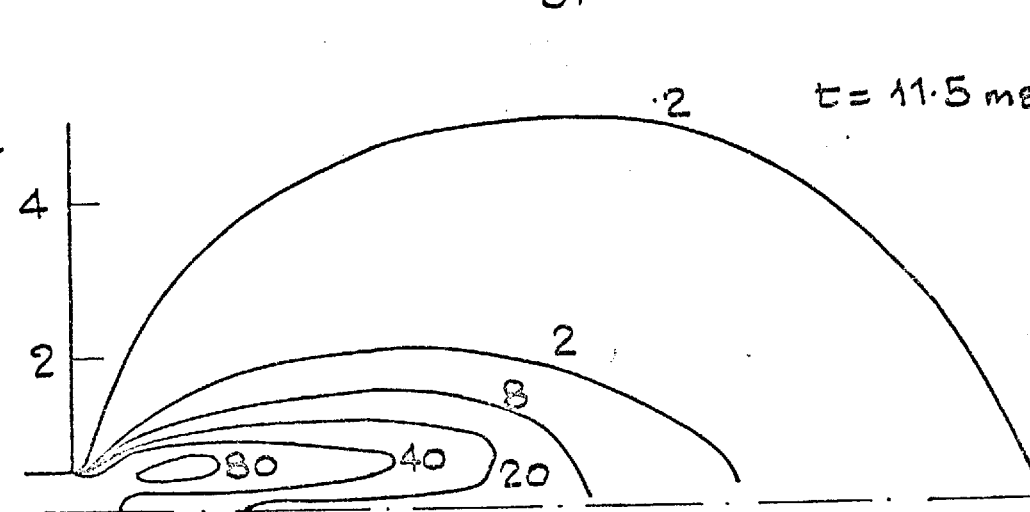
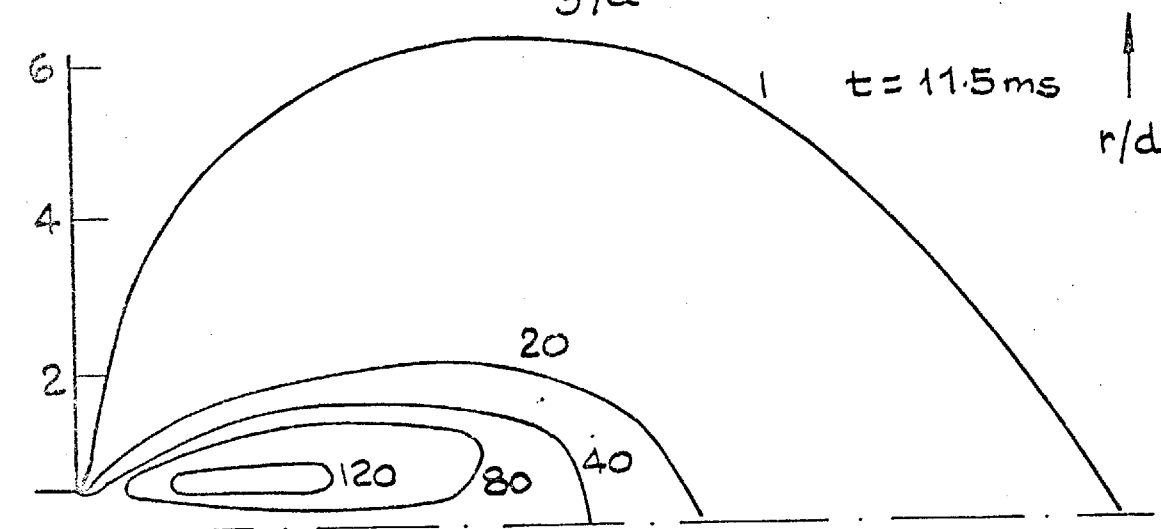
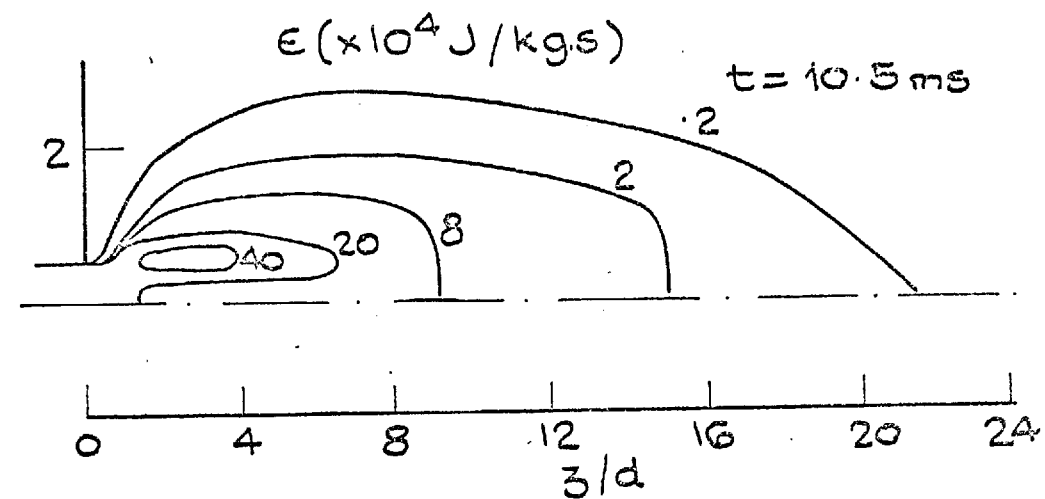
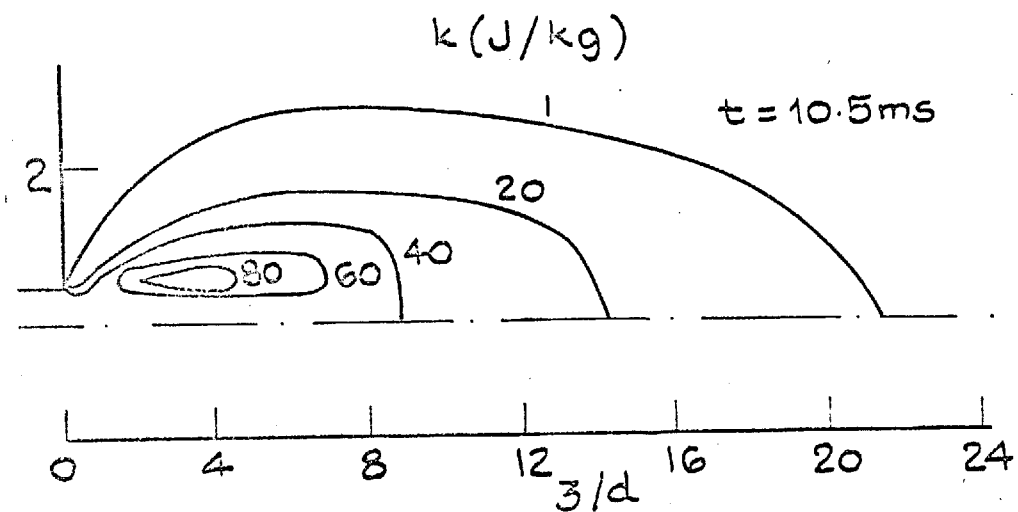


FIG. 3.6-10: DISTRIBUTIONS OF TURBULENT KINETIC ENERGY AND ITS DISSIPATION RATE AT TWO DIFFERENT TIME INTERVALS FOR IGNITION CASE.

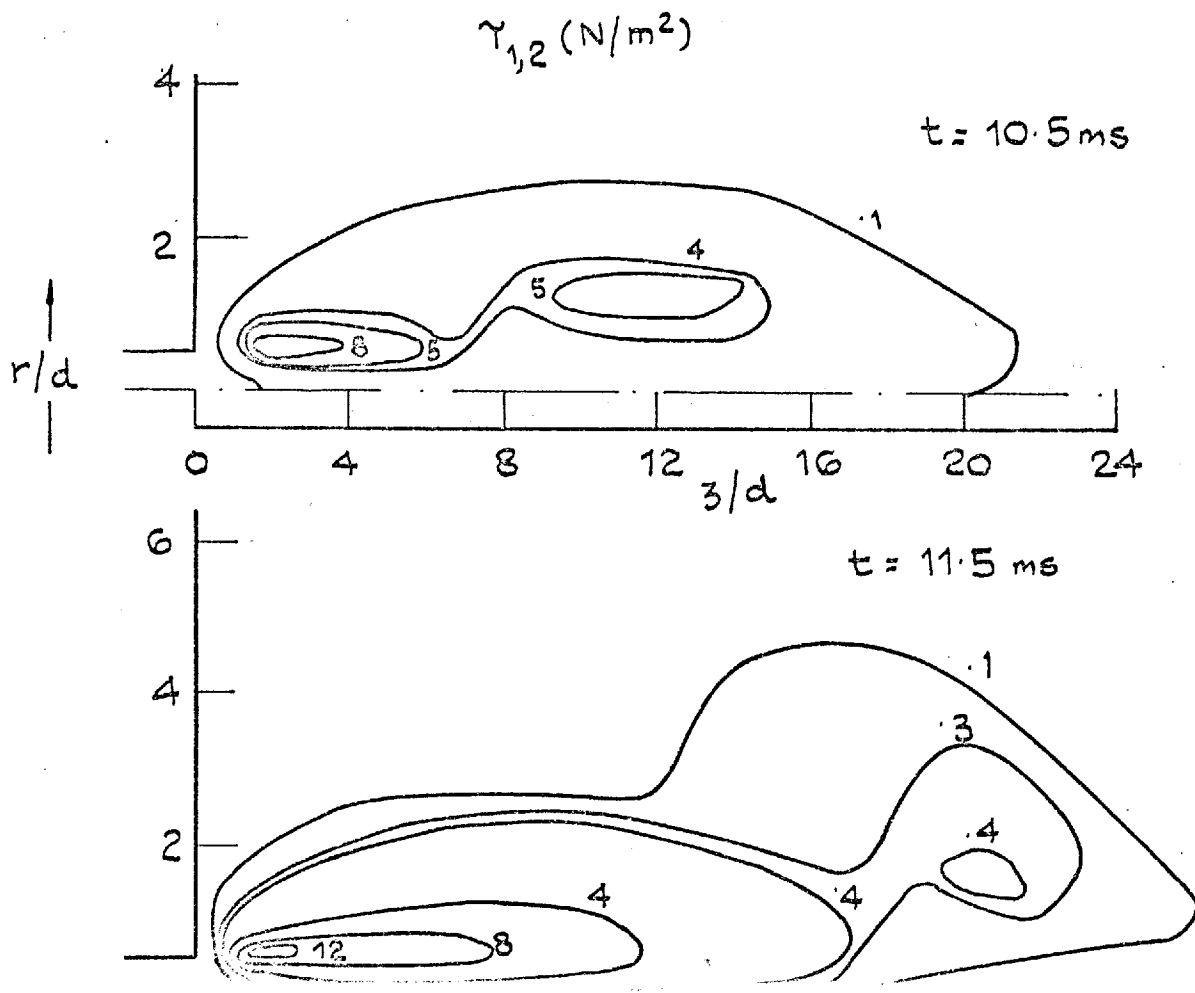


FIG. 3. G-11: DISTRIBUTION OF SHEAR STRESS
AT TWO DIFFERENT TIME-INTERVALS
FOR IGNITION CASE.

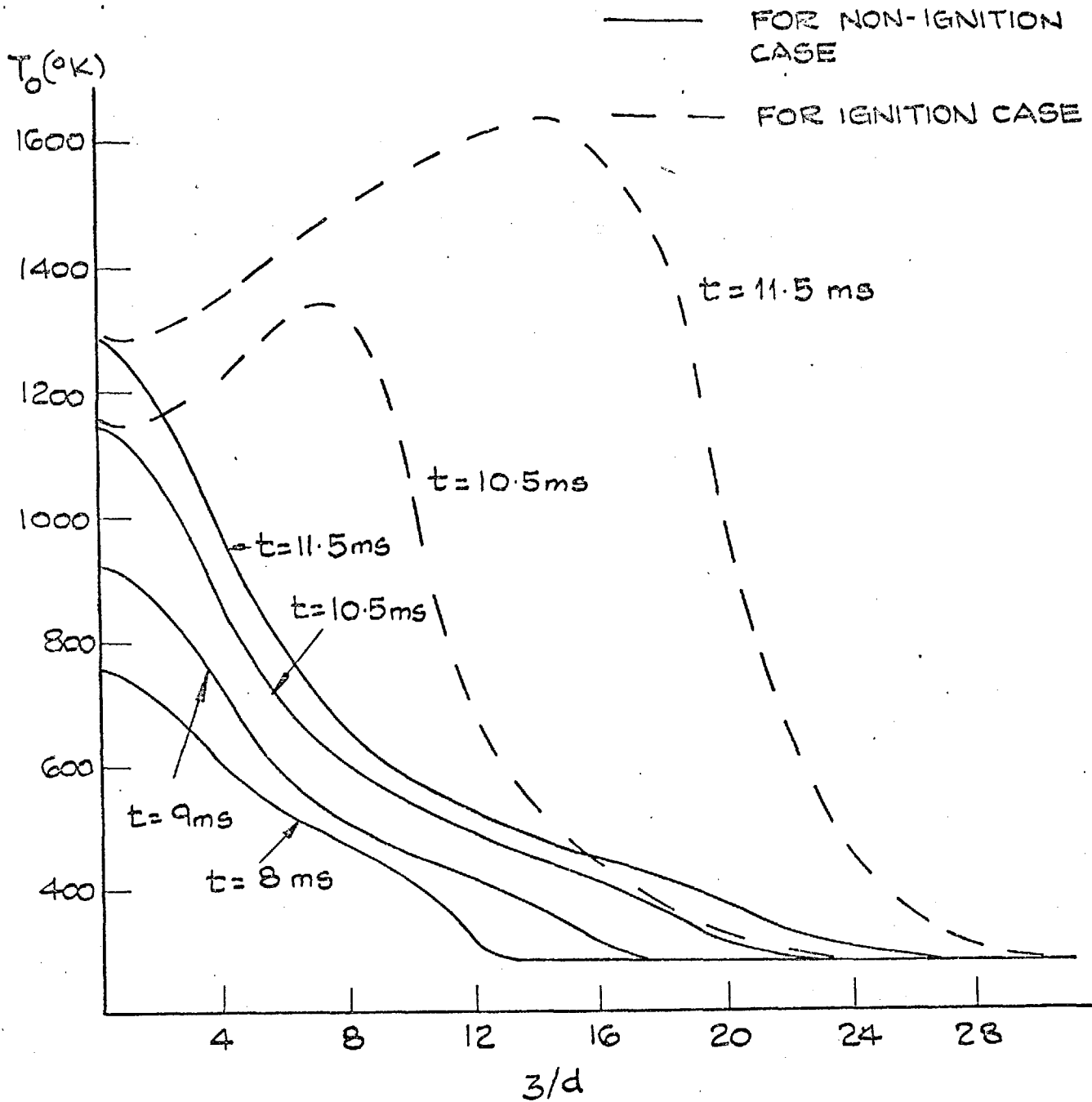


FIG.3.6-12: AXIAL TEMPERATURE DISTRIBUTION AT
DIFFERENT TIME - INTERVALS FOR IGNITION
AND NON-IGNITION CASES.

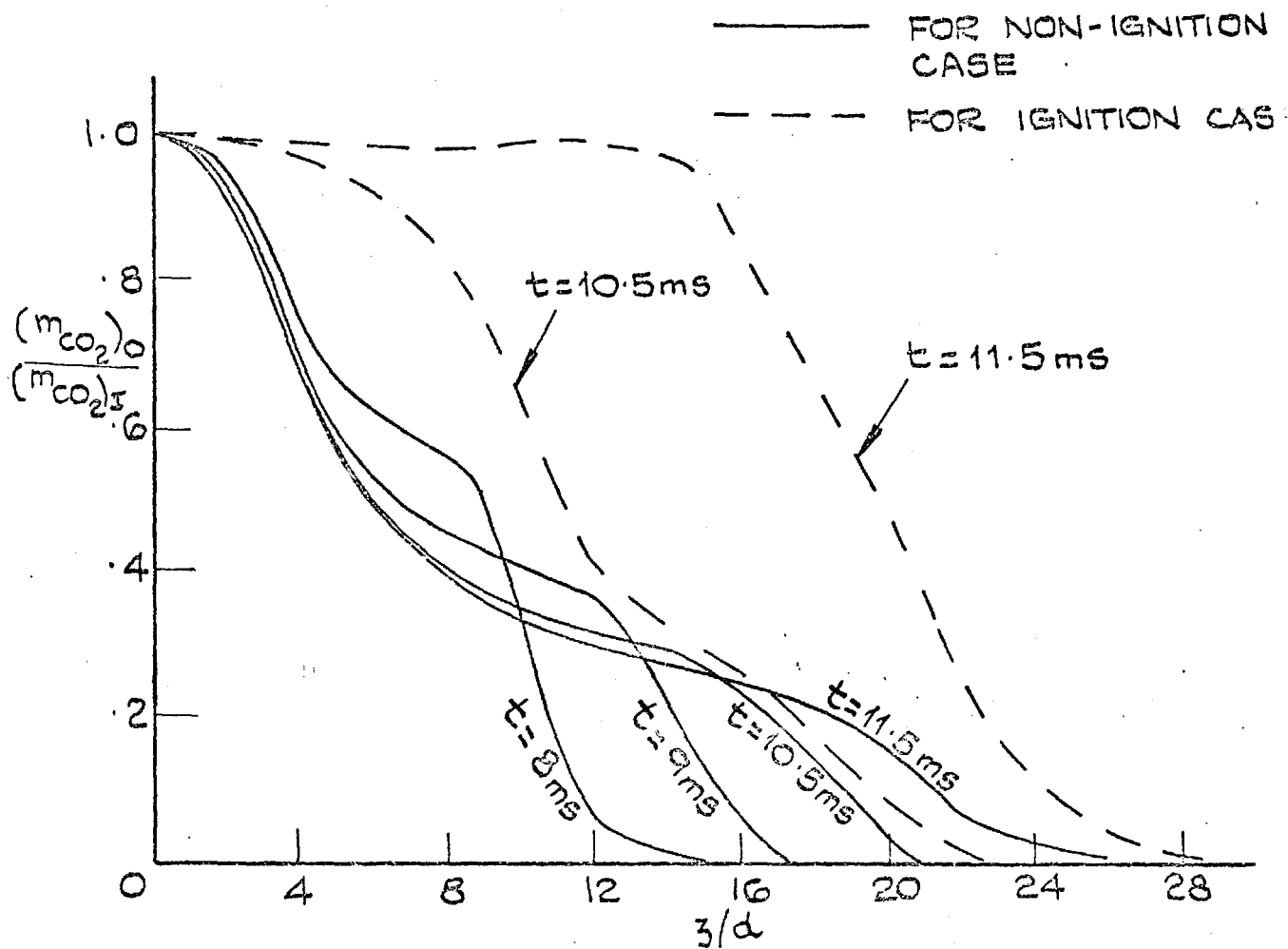
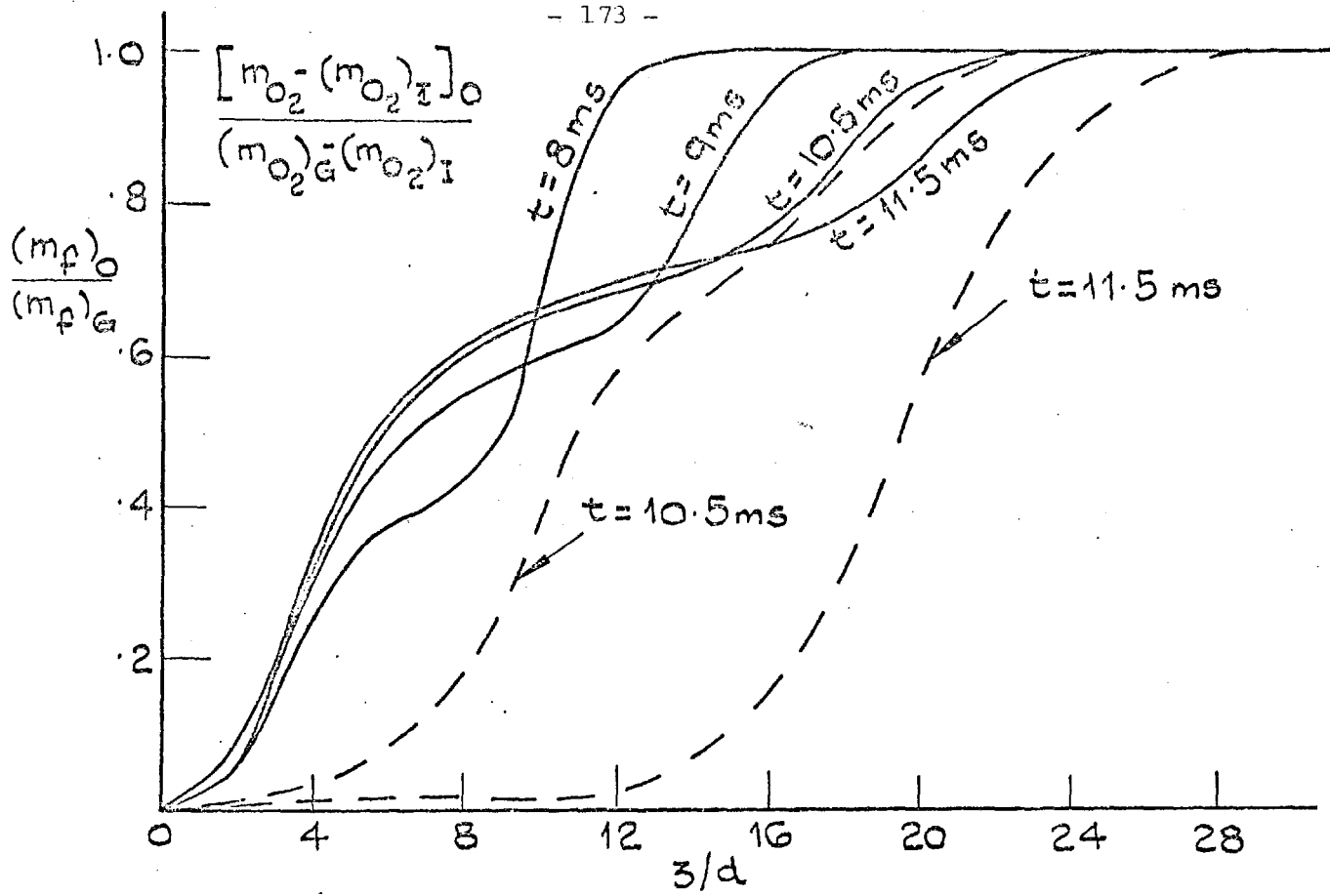


FIG.3.6-13: AXIAL CONCENTRATION DISTRIBUTIONS AT DIFFERENT TIME-INTERVALS FOR IGNITION AND NON-IGNITION CASES.

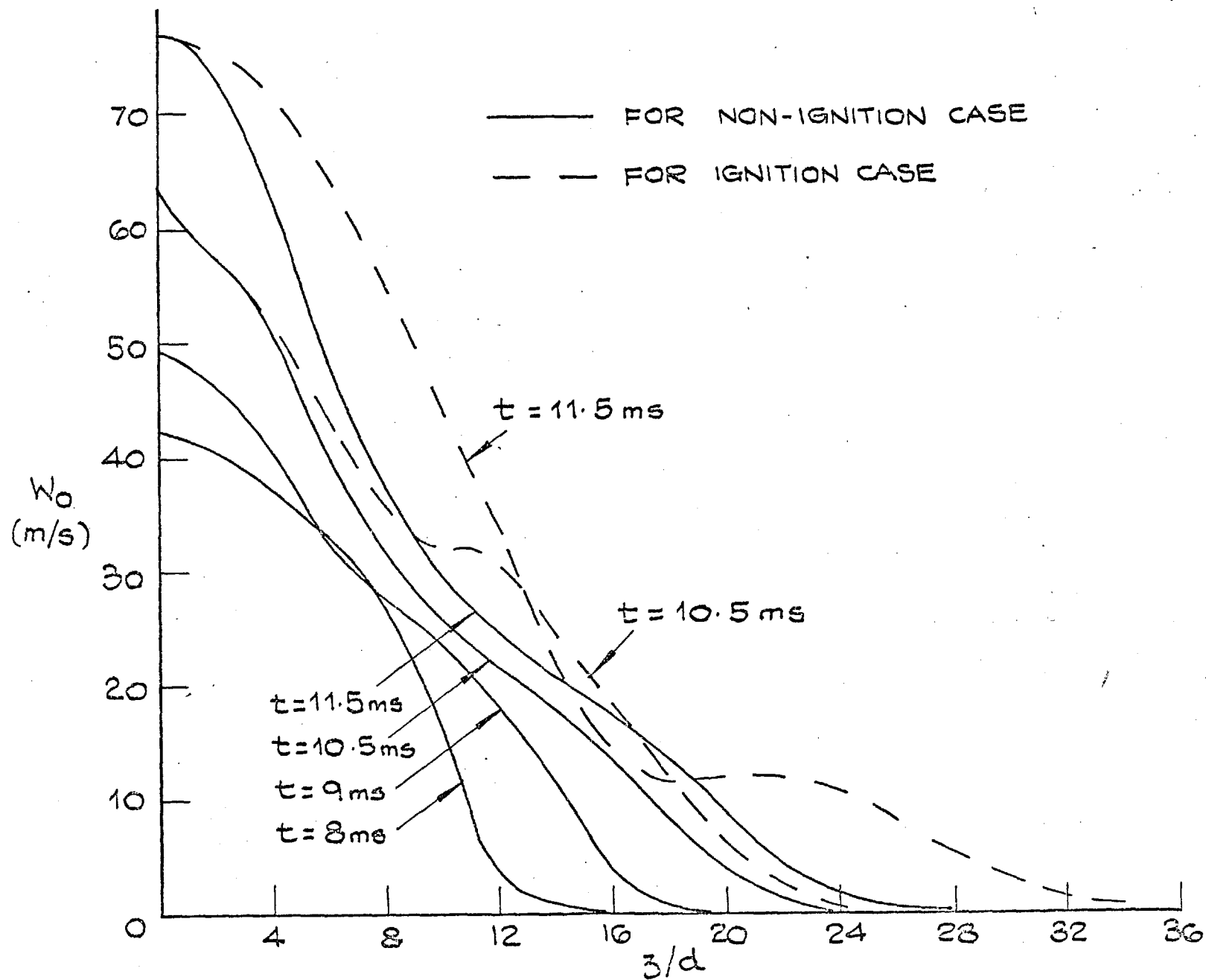


FIG.3.6-14:AXIAL DISTRIBUTION OF LONGITUDINAL VELOCITY AT DIFFERENT TIME - INTERVALS FOR IGNITION AND NON-IGNITION CASES.

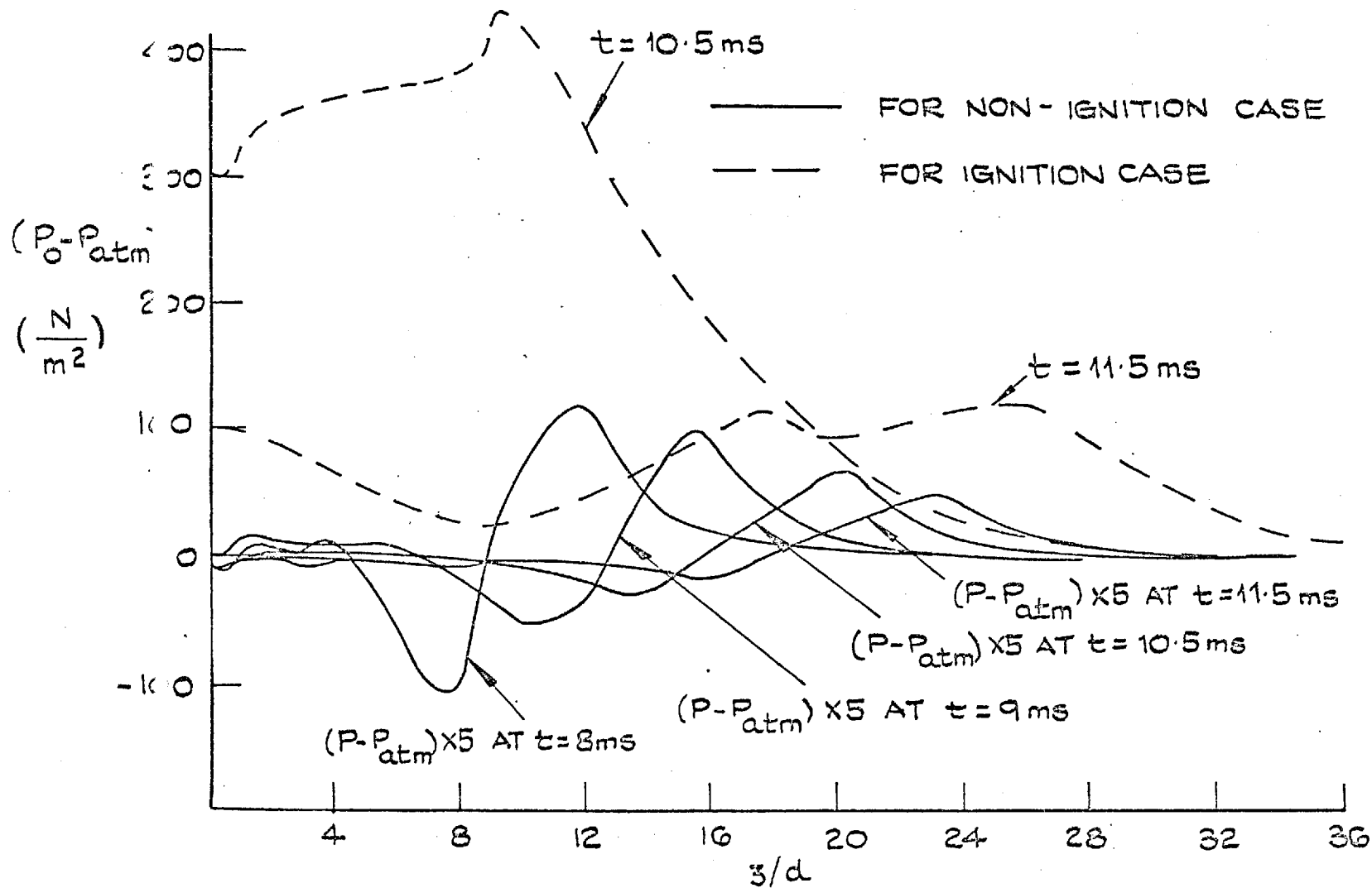


FIG. 3.6-15: AXIAL STATIC PRESSURE DISTRIBUTION AT DIFFERENT TIME-INTERVALS FOR IGNITION AND NON-IGNITION CASES.

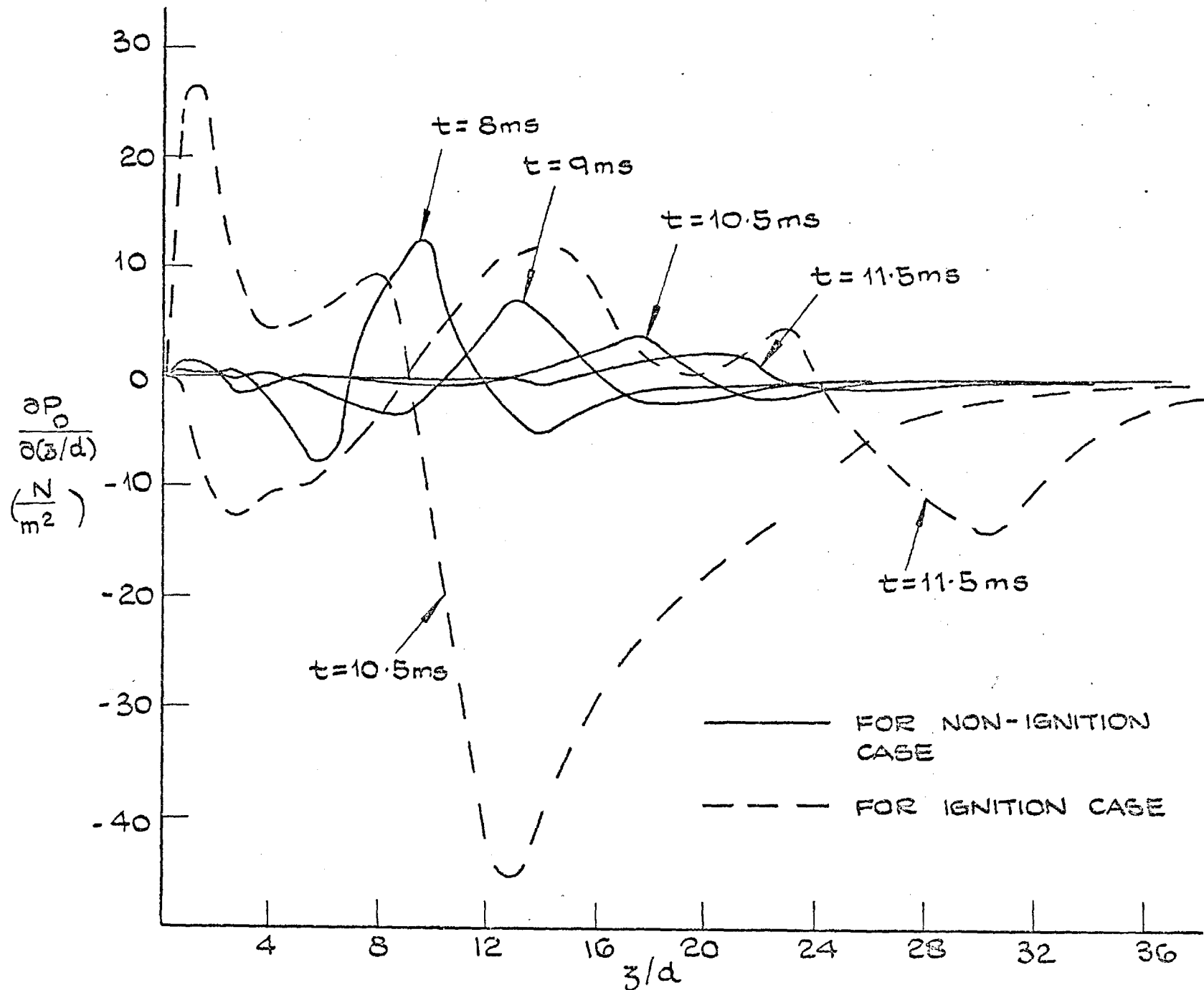


FIG.3.6-16: AXIAL DISTRIBUTION OF STATIC PRESSURE GRADIENT AT DIFFERENT TIME-INTERVALS FOR IGNITION AND NON-IGNITION CASES.

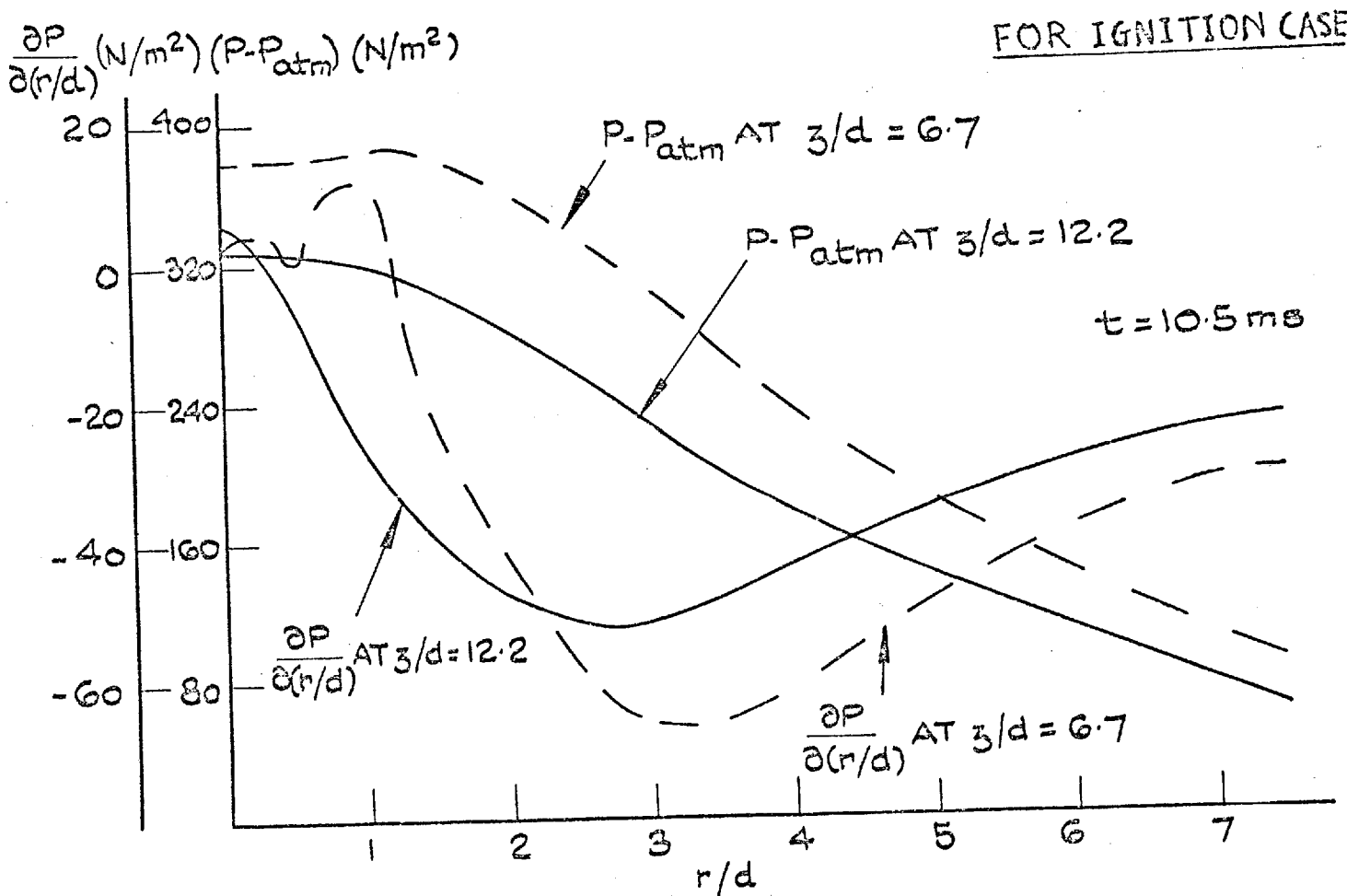
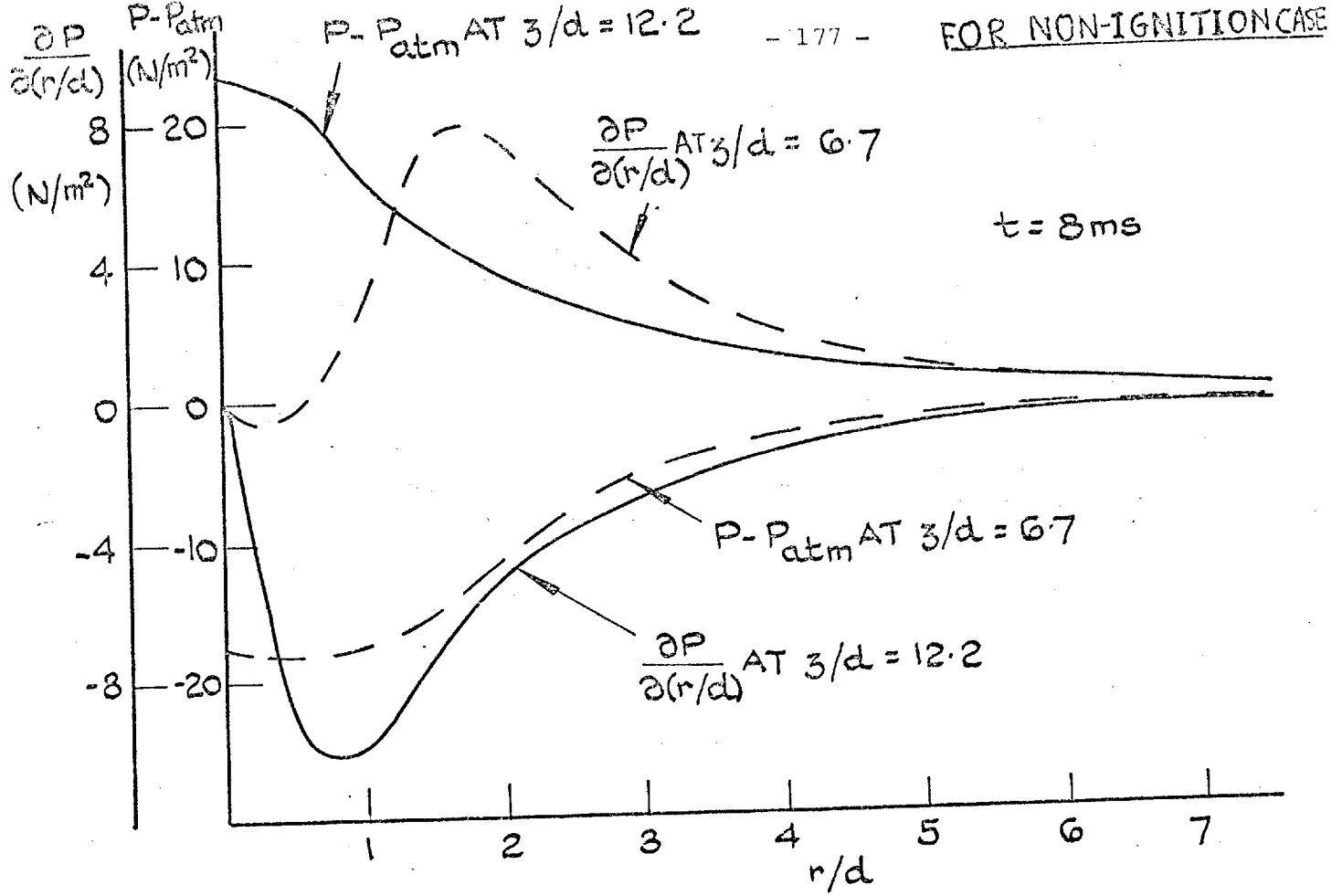


FIG. 3.6-17. RADIAL DISTRIBUTIONS OF STATIC PRESSURE AND PRESSURE GRADIENT AT TWO DIFFERENT LOCATIONS AND TIME INTERVALS.

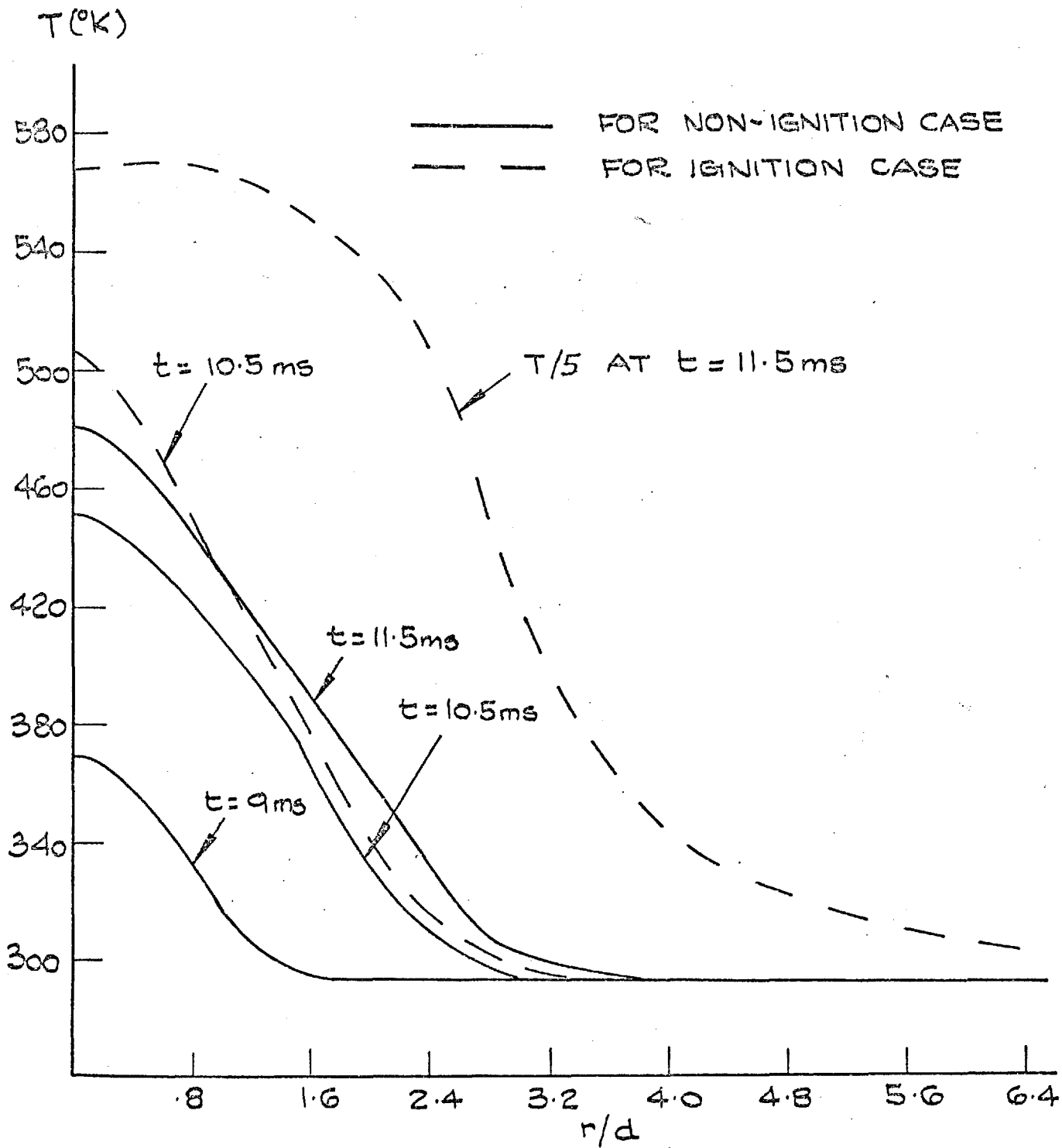


FIG. 3.6-18: RADIAL DISTRIBUTION OF TEMPERATURE
AT $3/d = 14.25$ AND AT DIFFERENT
TIME-INTERVALS FOR IGNITION AND
NON-IGNITION CASES.

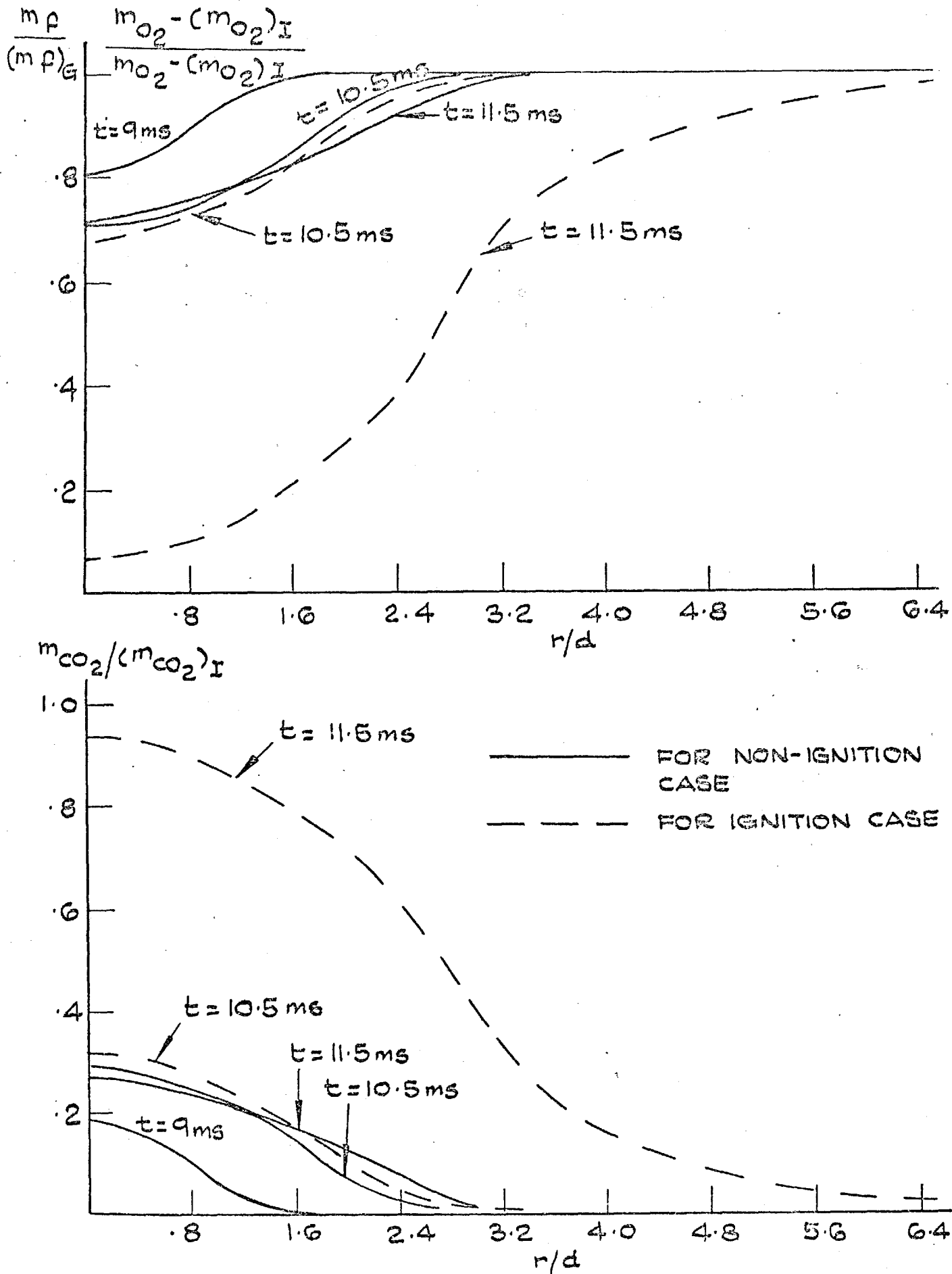


FIG. 3.6-19 : RADIAL CONCENTRATION DISTRIBUTIONS AT $3/d = 14.25$ AND AT DIFFERENT TIME-INTERVALS FOR IGNITION AND NON-IGNITION CASES.

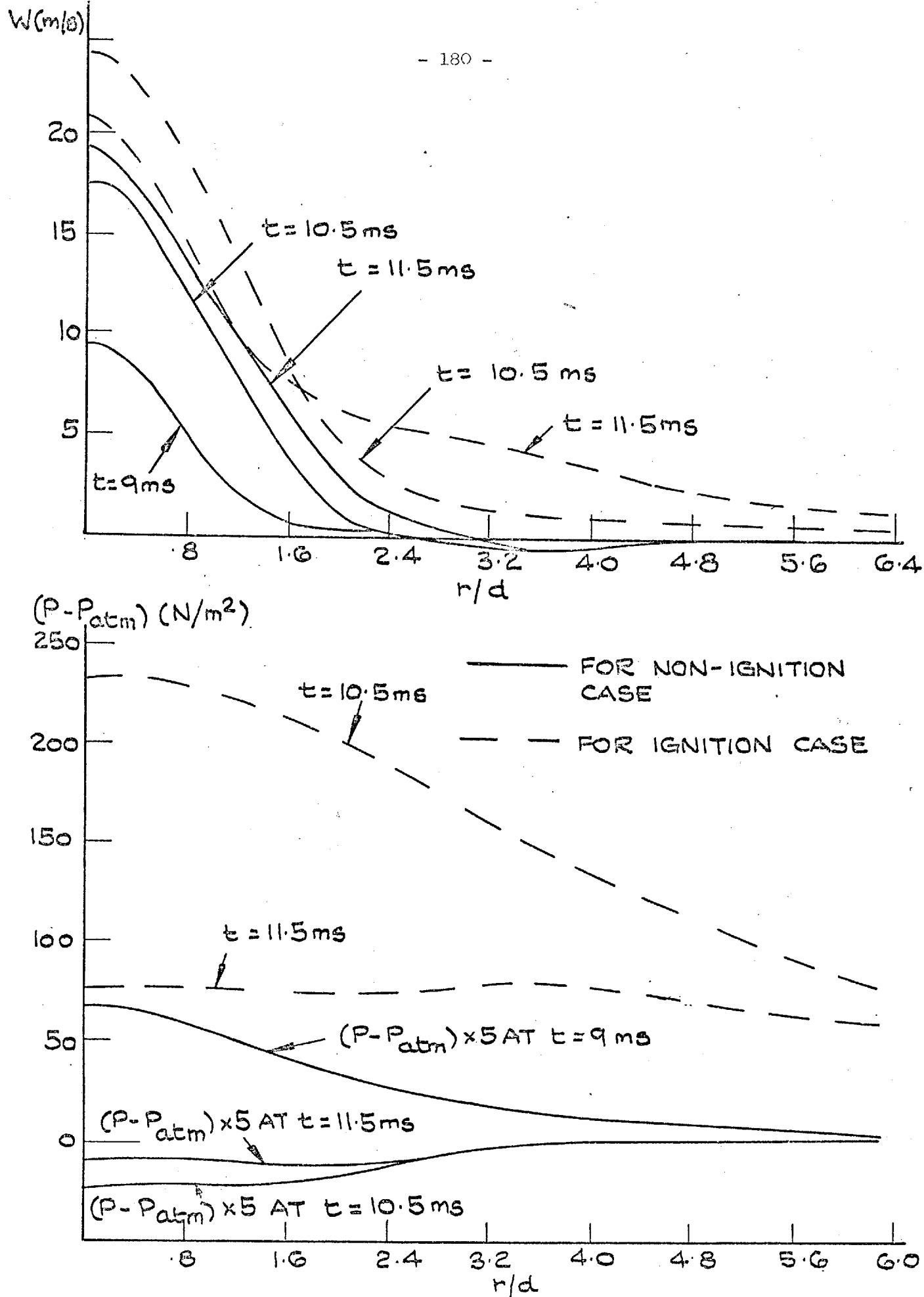


FIG. 3.6-20: RADIAL DISTRIBUTIONS OF LONGITUDINAL VELOCITY AND STATIC PRESSURE AT $z/d=4.25$ AND AT DIFFERENT TIME-INTERVALS FOR IGNITION AND NON-IGNITION CASES.

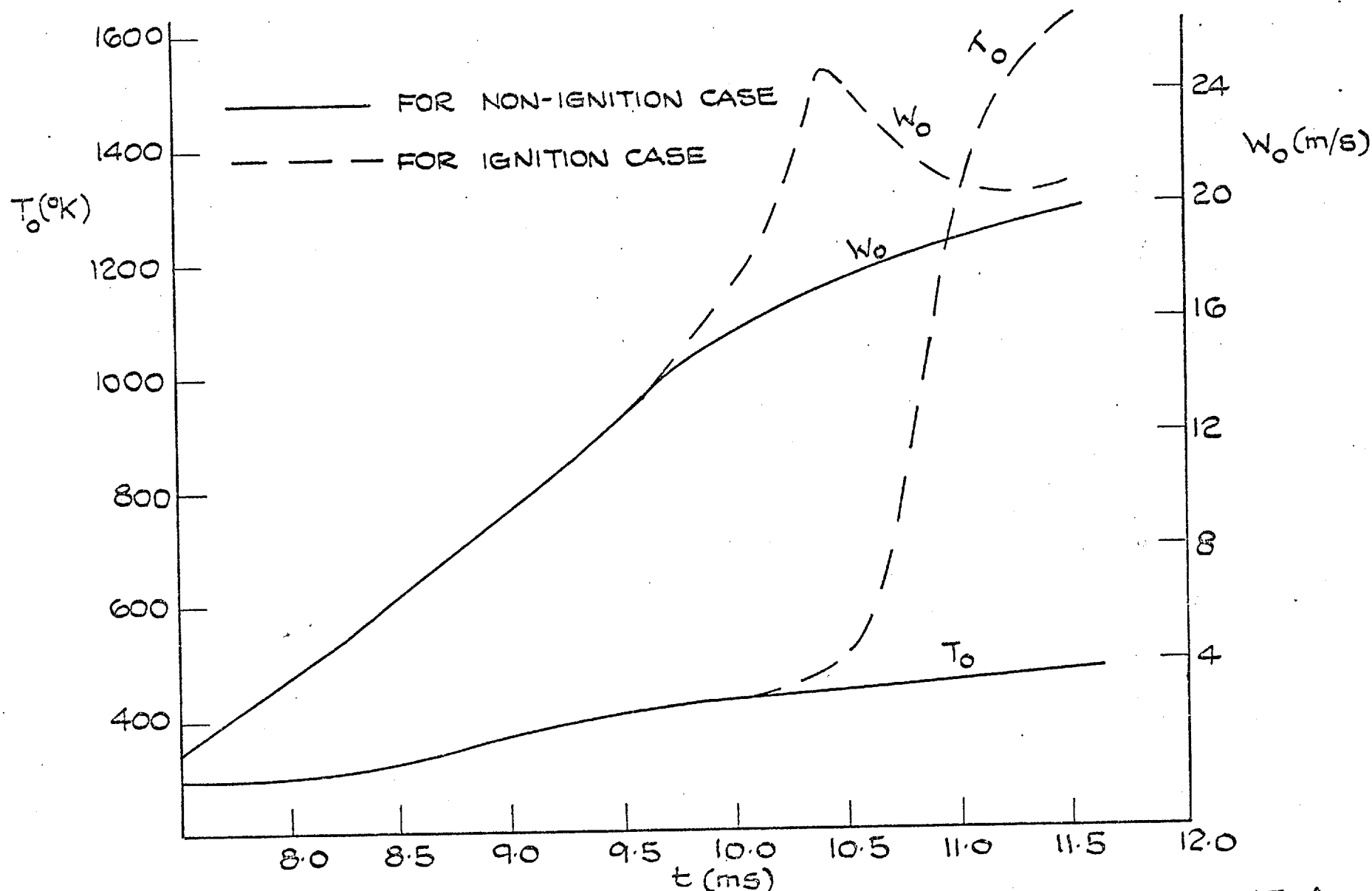


FIG. 3.6-21: DEVELOPMENTS OF TEMPERATURE AND LONGITUDINAL VELOCITY AT A POINT ON THE JET AXIS 14.25d FROM THE NOZZLE OUTLET FOR IGNITION AND NON-IGNITION CASES.

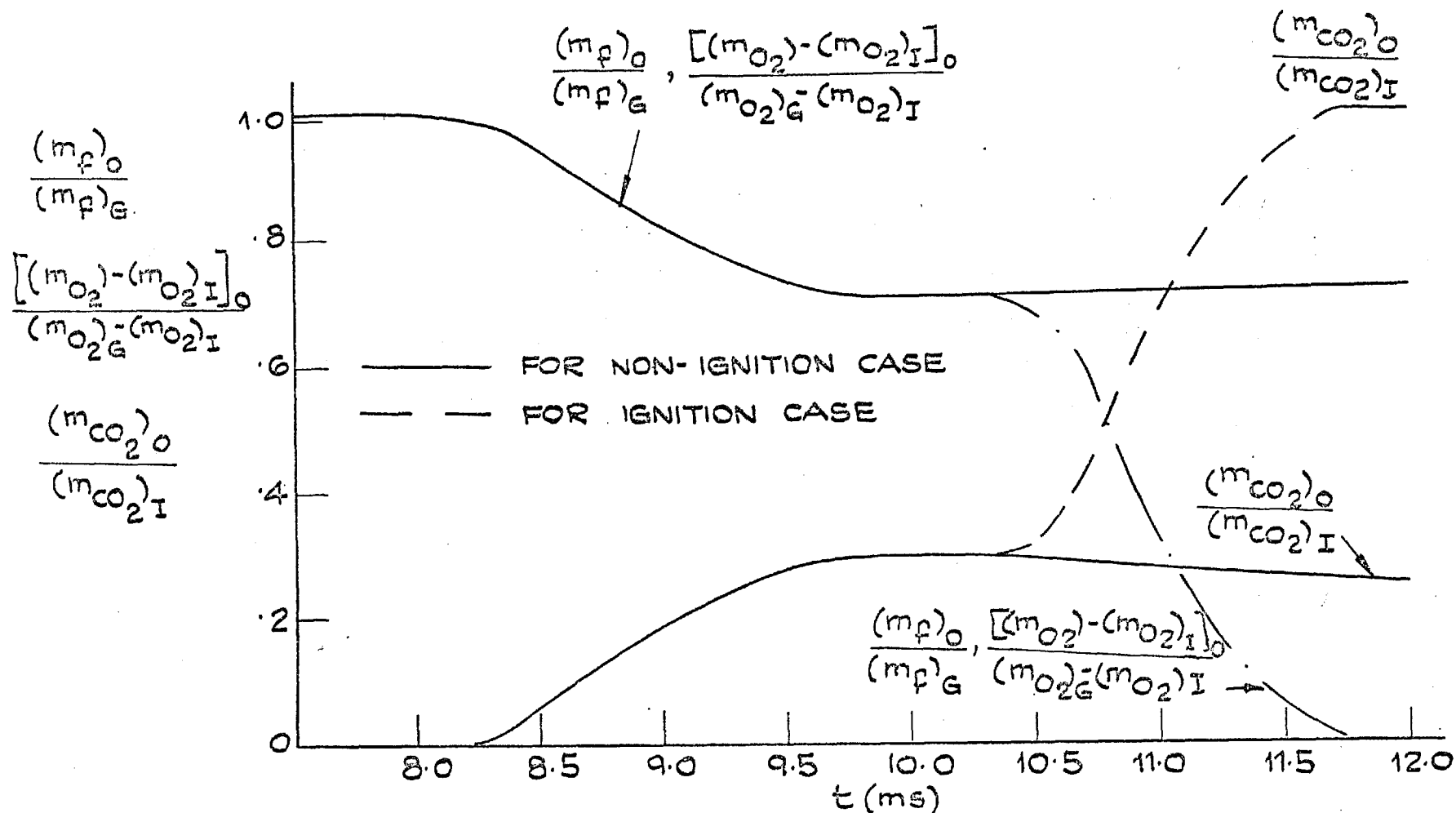


FIG. 3.6-22: DEVELOPMENTS OF SPECIES CONCENTRATIONS AT A POINT ON THE JET AXIS 14.25 d FROM THE NOZZLE OUTLET FOR IGNITION AND NON-IGNITION CASES.

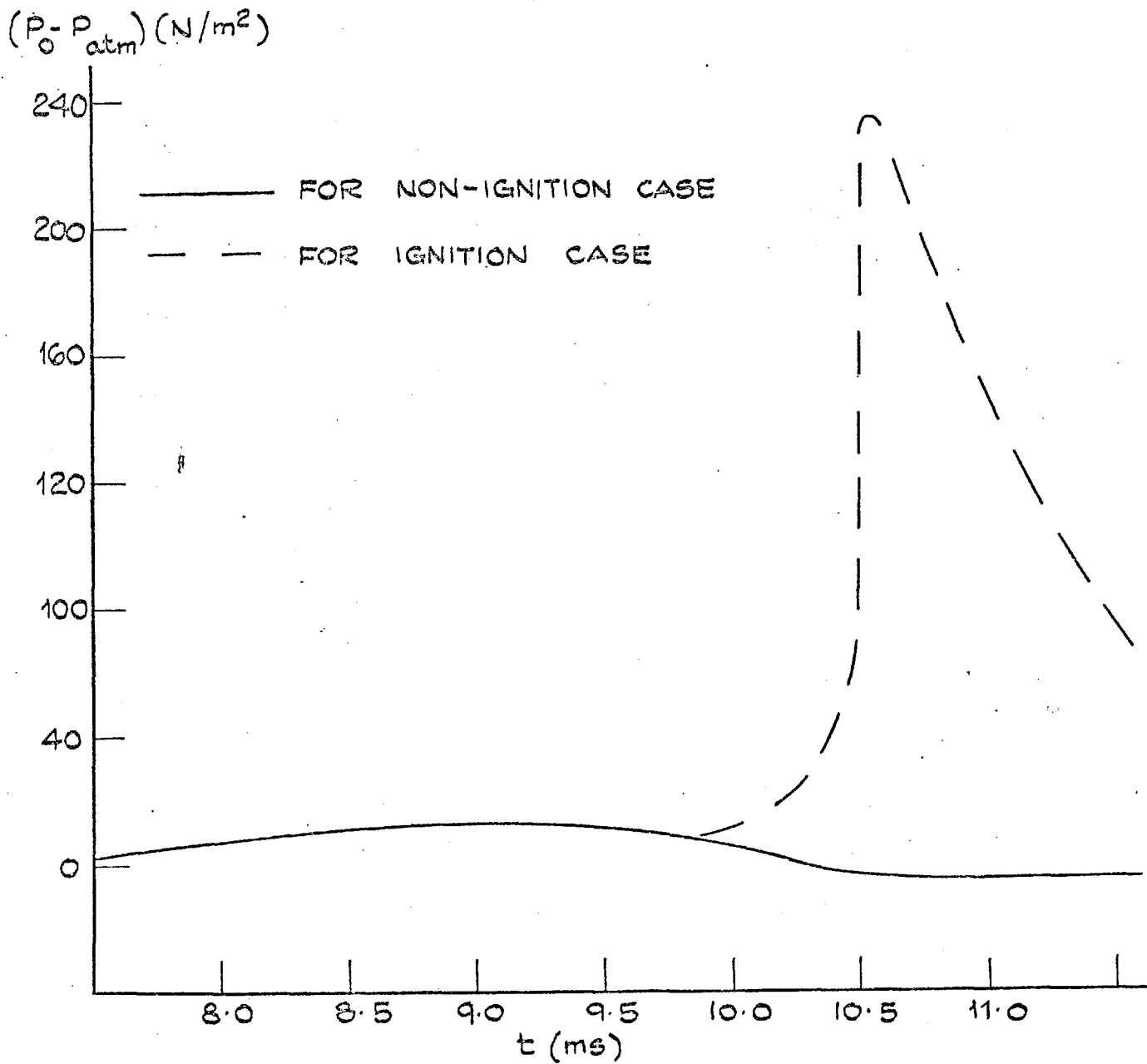


FIG. 3.6-23: DEVELOPMENT OF STATIC PRESSURE AT A
POINT ON THE JET AXIS 14.25 d FROM
THE NOZZLE ORIFICE FOR IGNITION AND
NON-IGNITION CASES.

$T (^{\circ}K)$

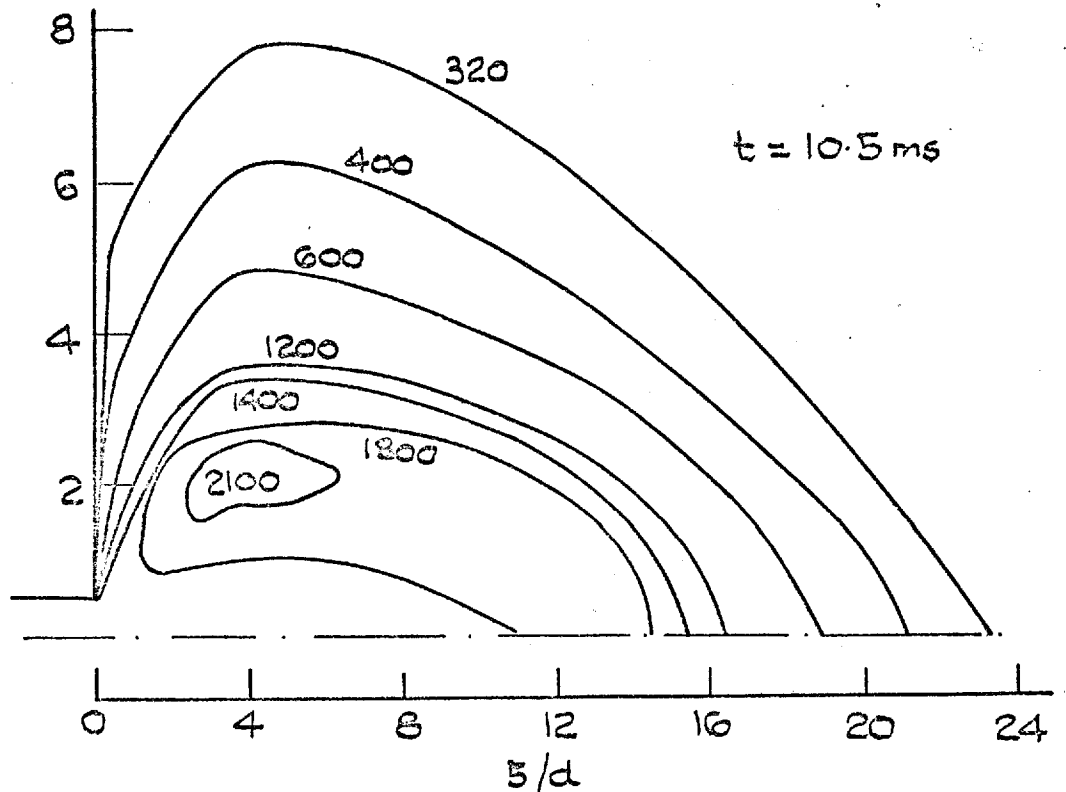
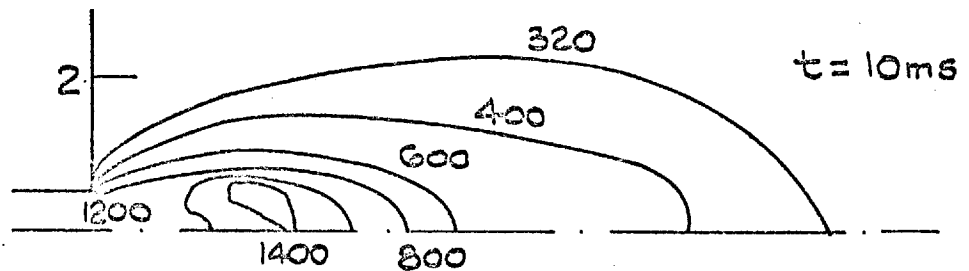
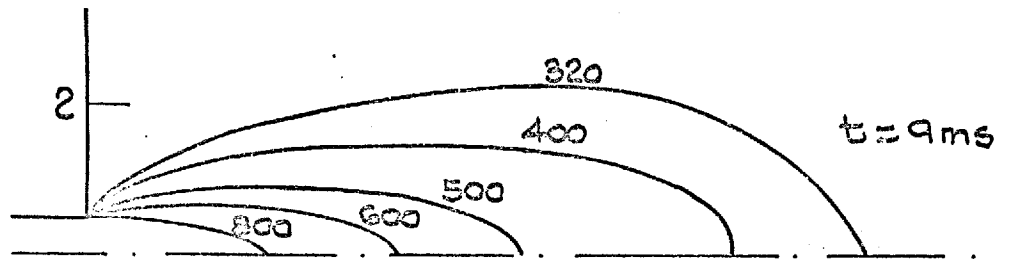


FIG. 3.6-24: DISTRIBUTION OF TEMPERATURE AT THREE DIFFERENT TIME-INTERVALS FOR IGNITION CASE WITH REACTION RATE PRESCRIBED BY ARRHENIUS' EXPRESSION ONLY.

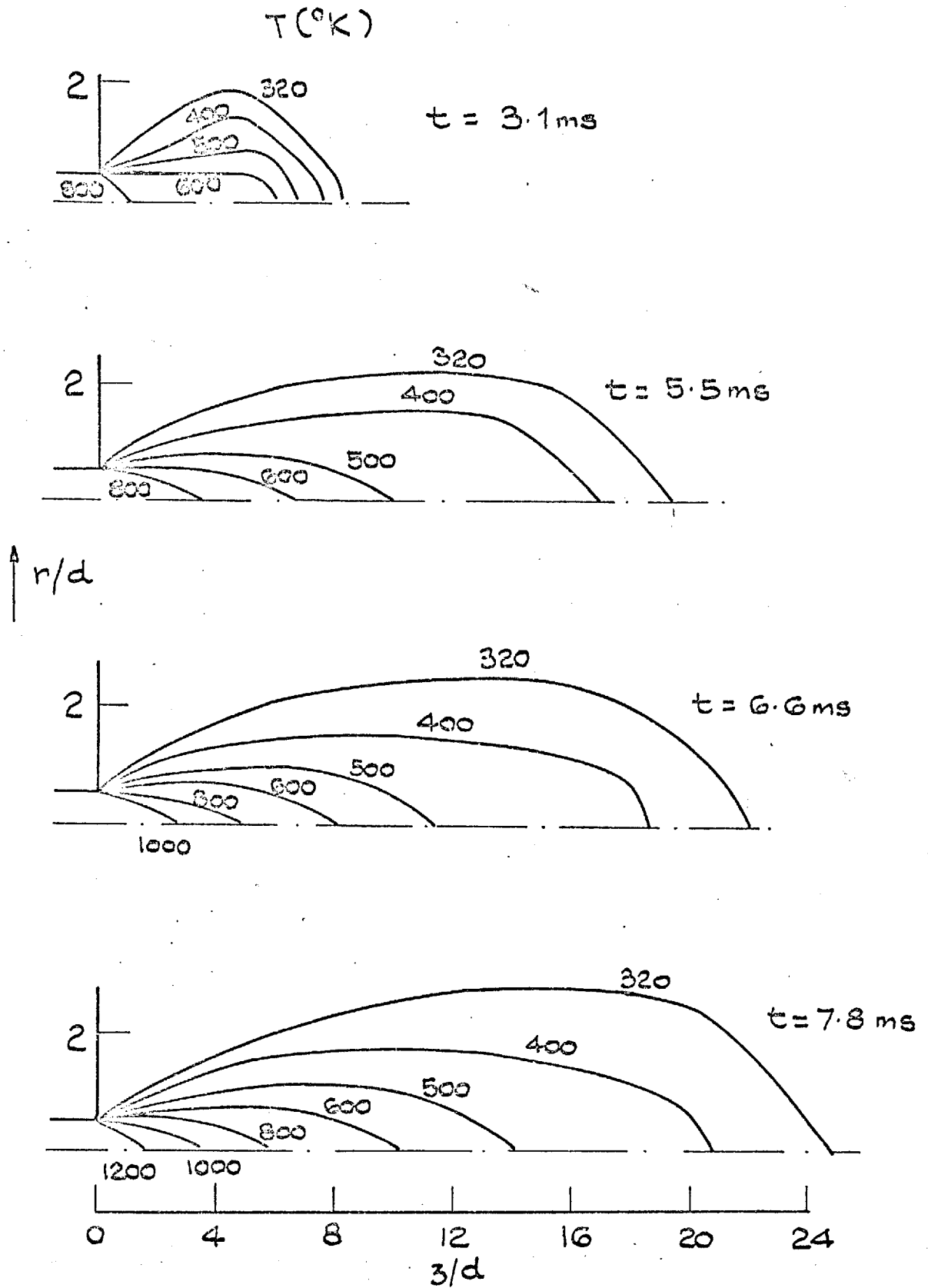


FIG. 3.6-25: DISTRIBUTION OF TEMPERATURE AT
FOUR DIFFERENT TIME-INTERVALS.

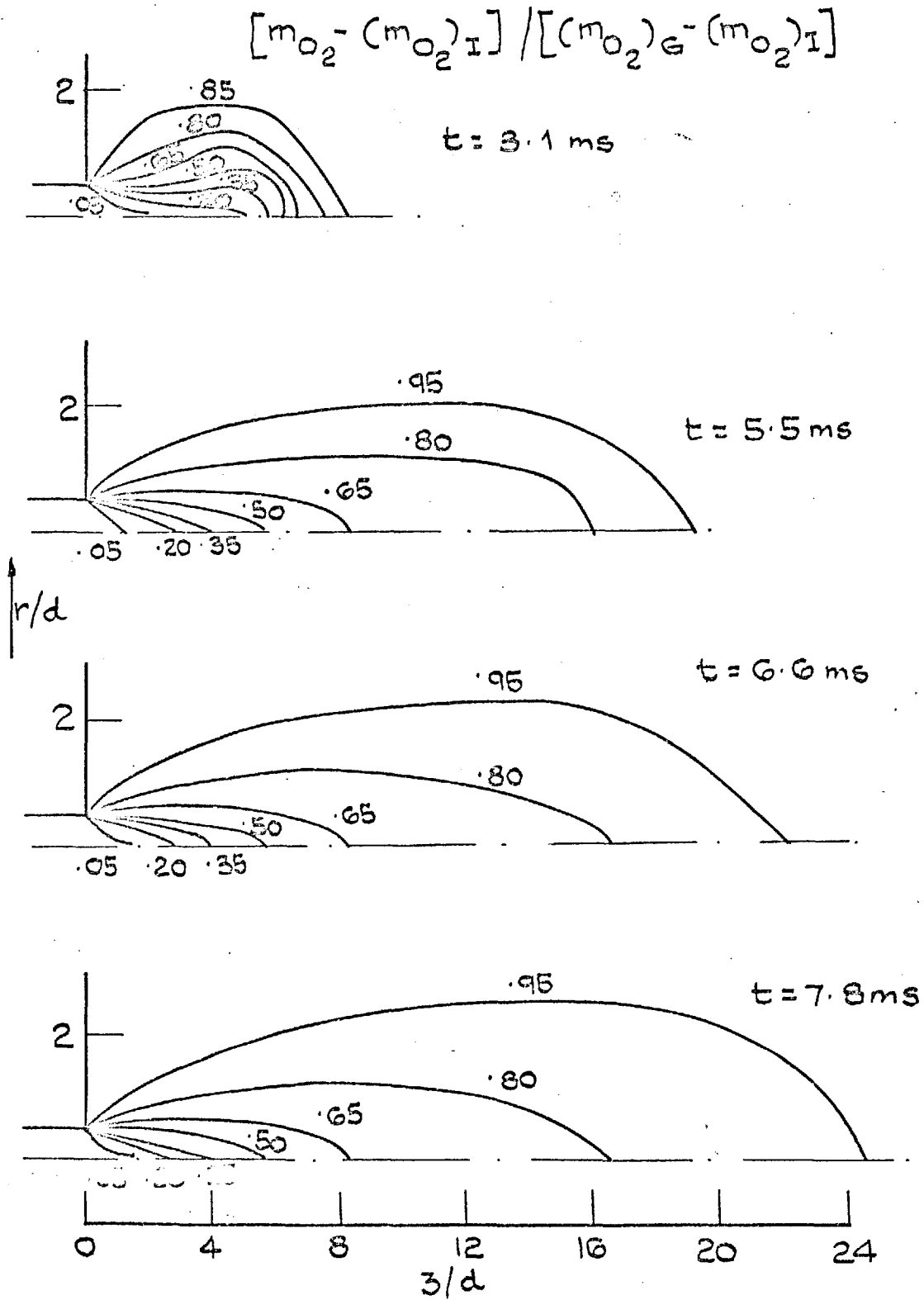


FIG. 3.6-26: DISTRIBUTION OF OXYGEN CONCENTRATION
AT FOUR DIFFERENT TIME-INTERVALS.

VELOCITY VECTOR (m/s)

2 m/s

SCALE: 

50 m/s



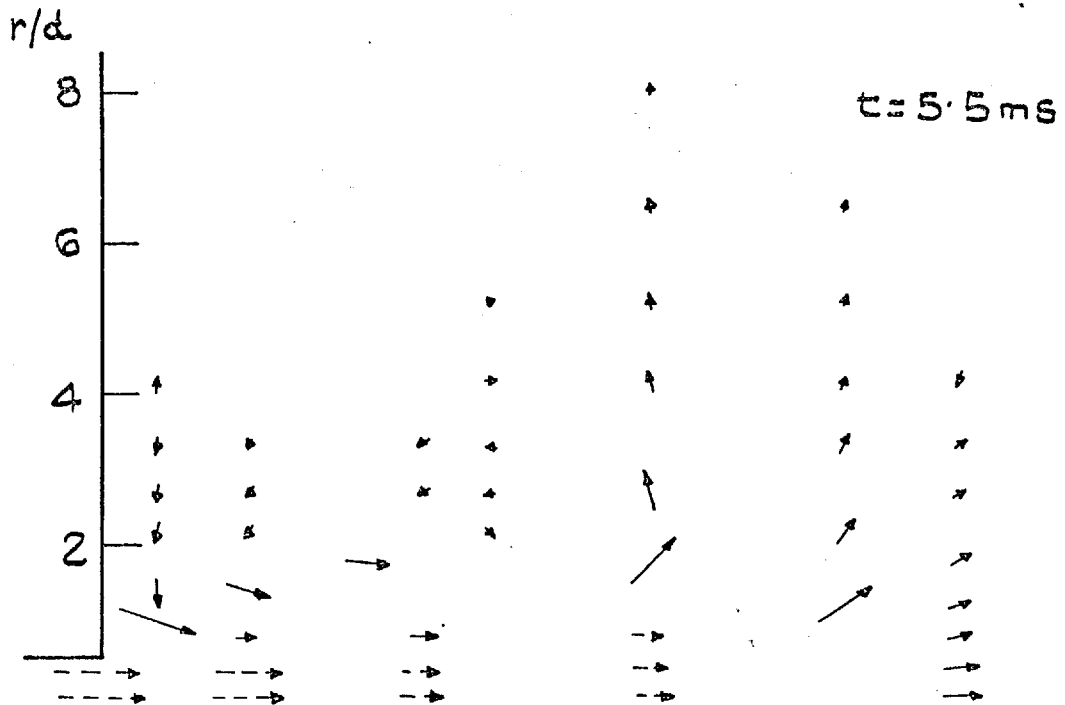
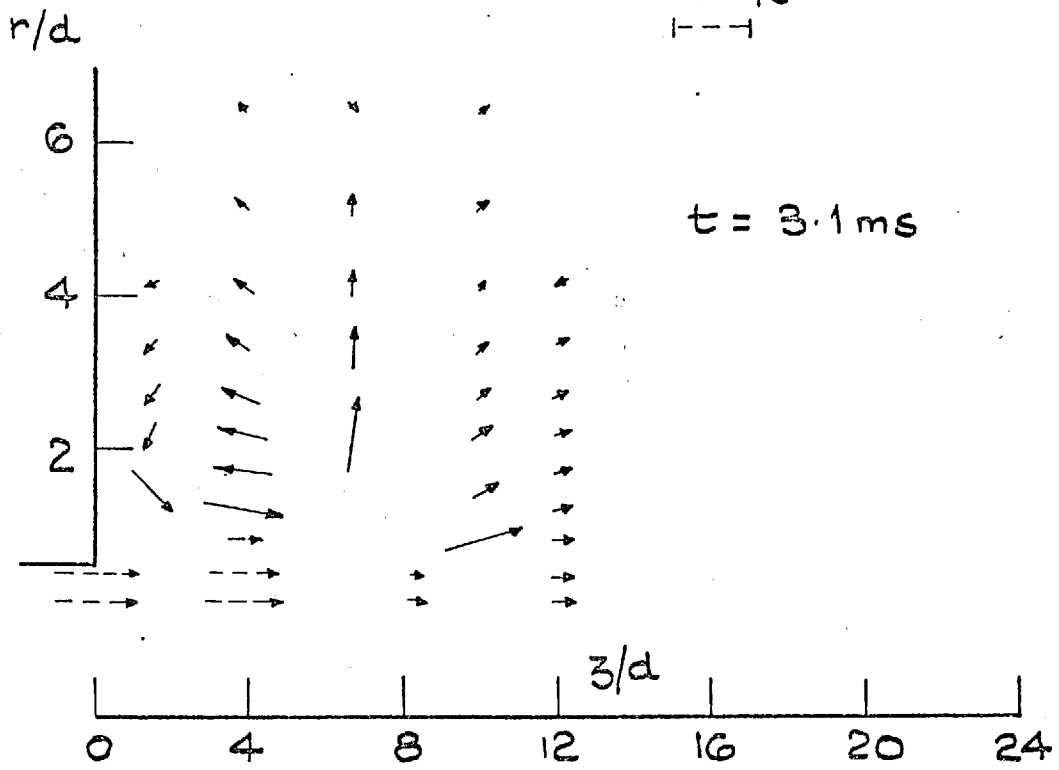


FIG. 3.6-27: VELOCITY-VECTOR DISTRIBUTION AT TWO DIFFERENT TIME-INTERVALS.

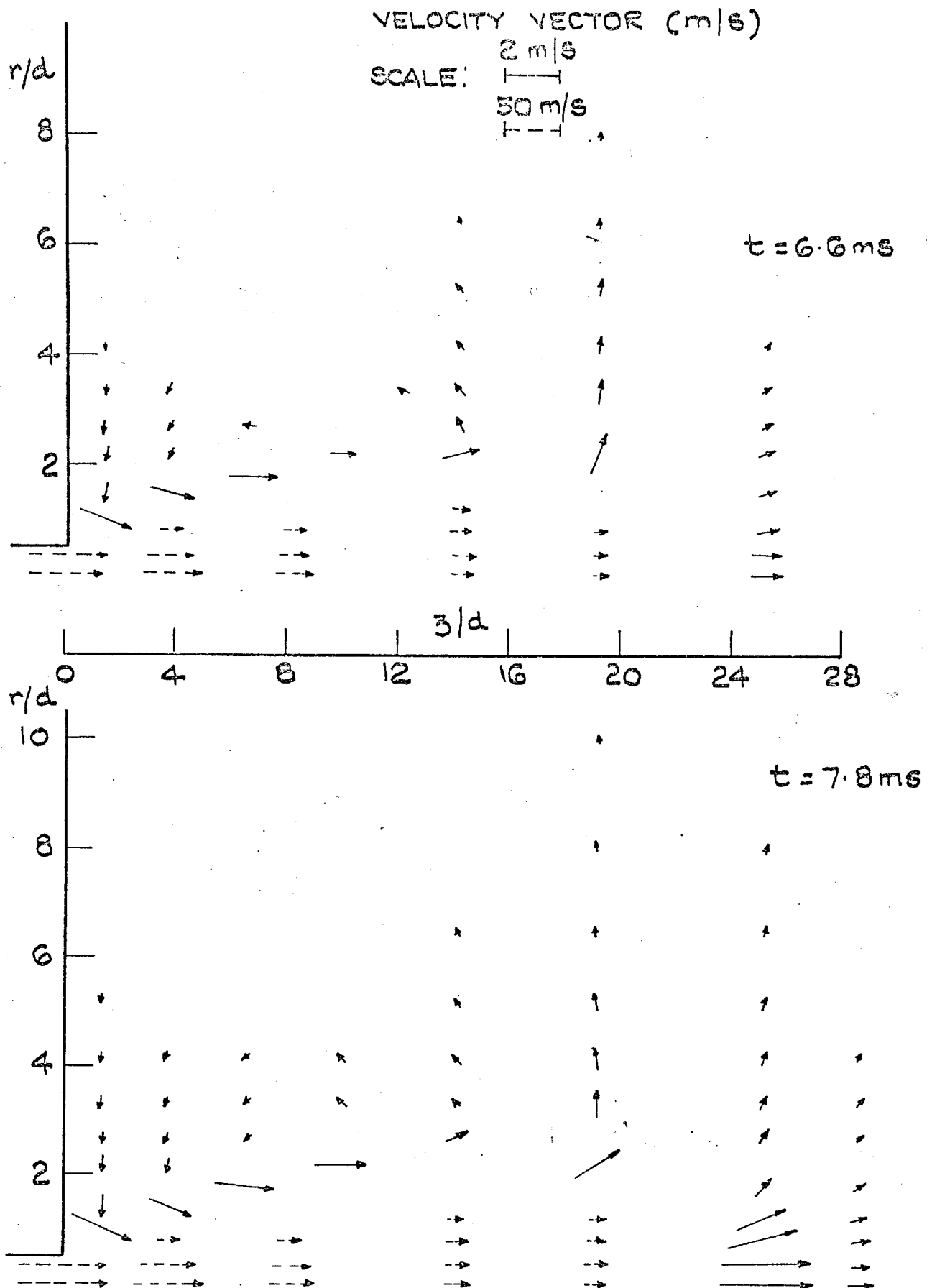


FIG. 3.6-28: VELOCITY - VECTOR DISTRIBUTION AT TWO DIFFERENT TIME-INTERVALS.

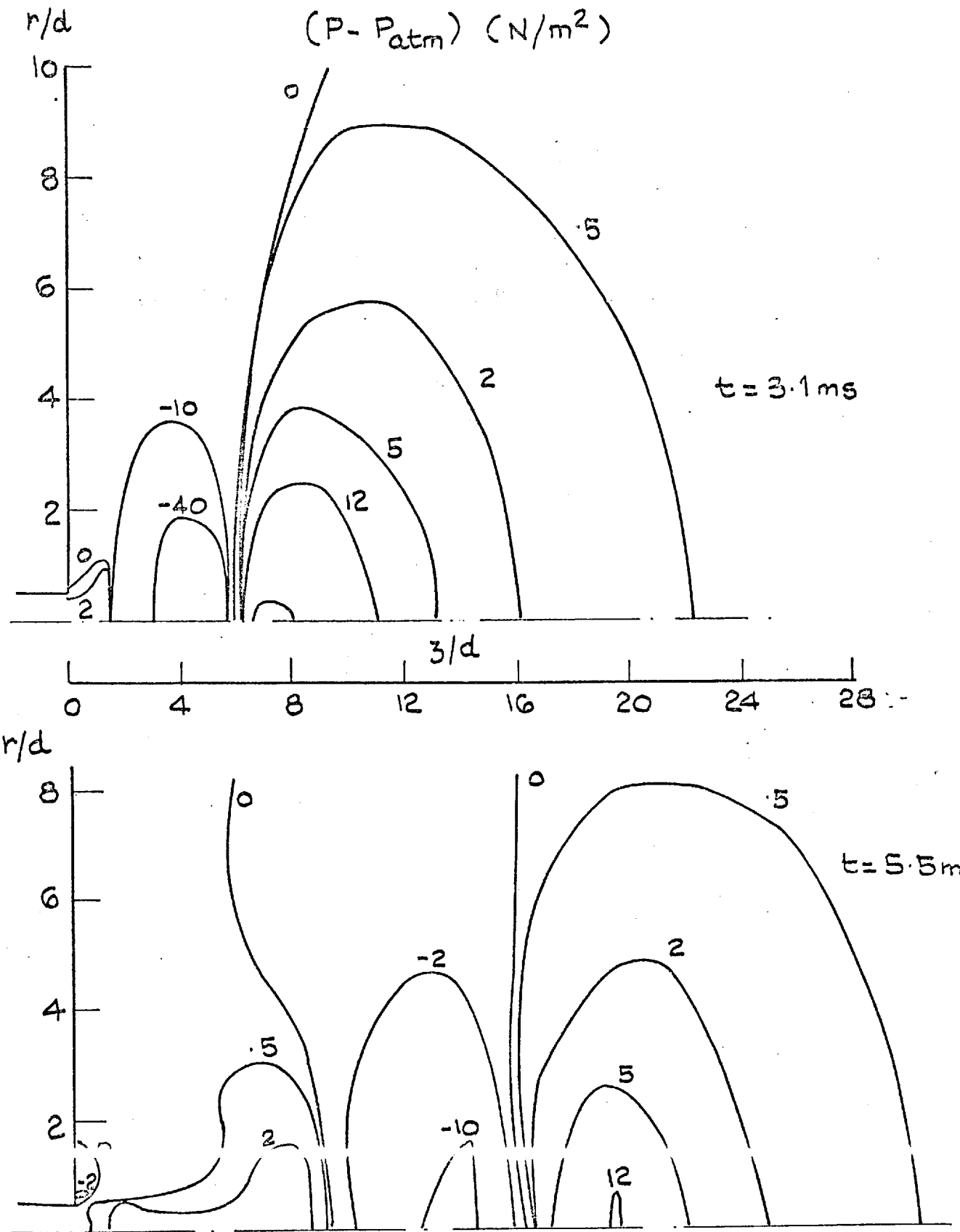


FIG. 3.6-29: STATIC PRESSURE DISTRIBUTION AT TWO DIFFERENT TIME - INTERVALS.

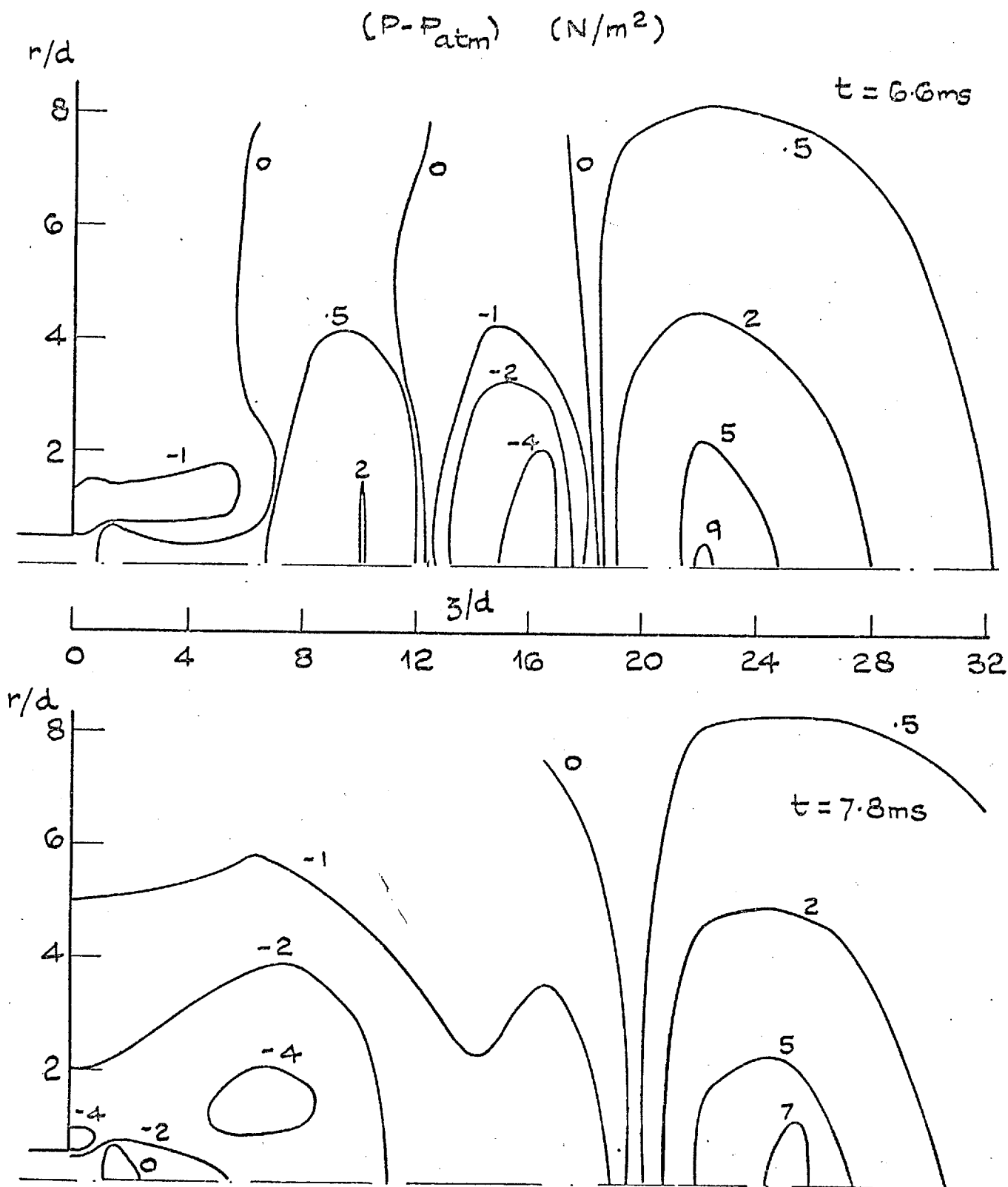


FIG. 3.6-30: STATIC PRESSURE DISTRIBUTION AT TWO DIFFERENT TIME - INTERVALS .

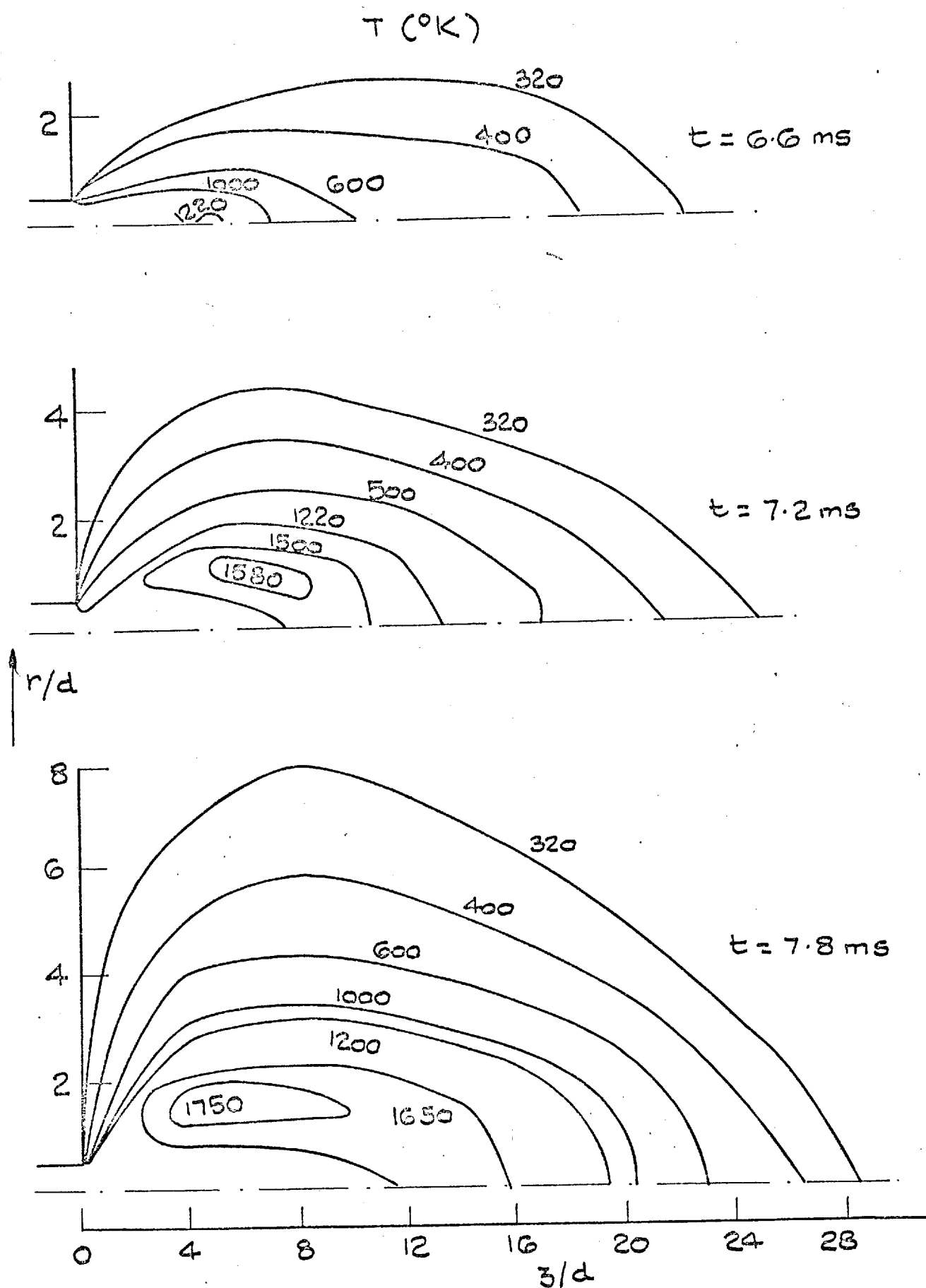


FIG. 3.6-31: DISTRIBUTION OF TEMPERATURE AT
THREE DIFFERENT TIME INTERVALS
WITH IGNITION.

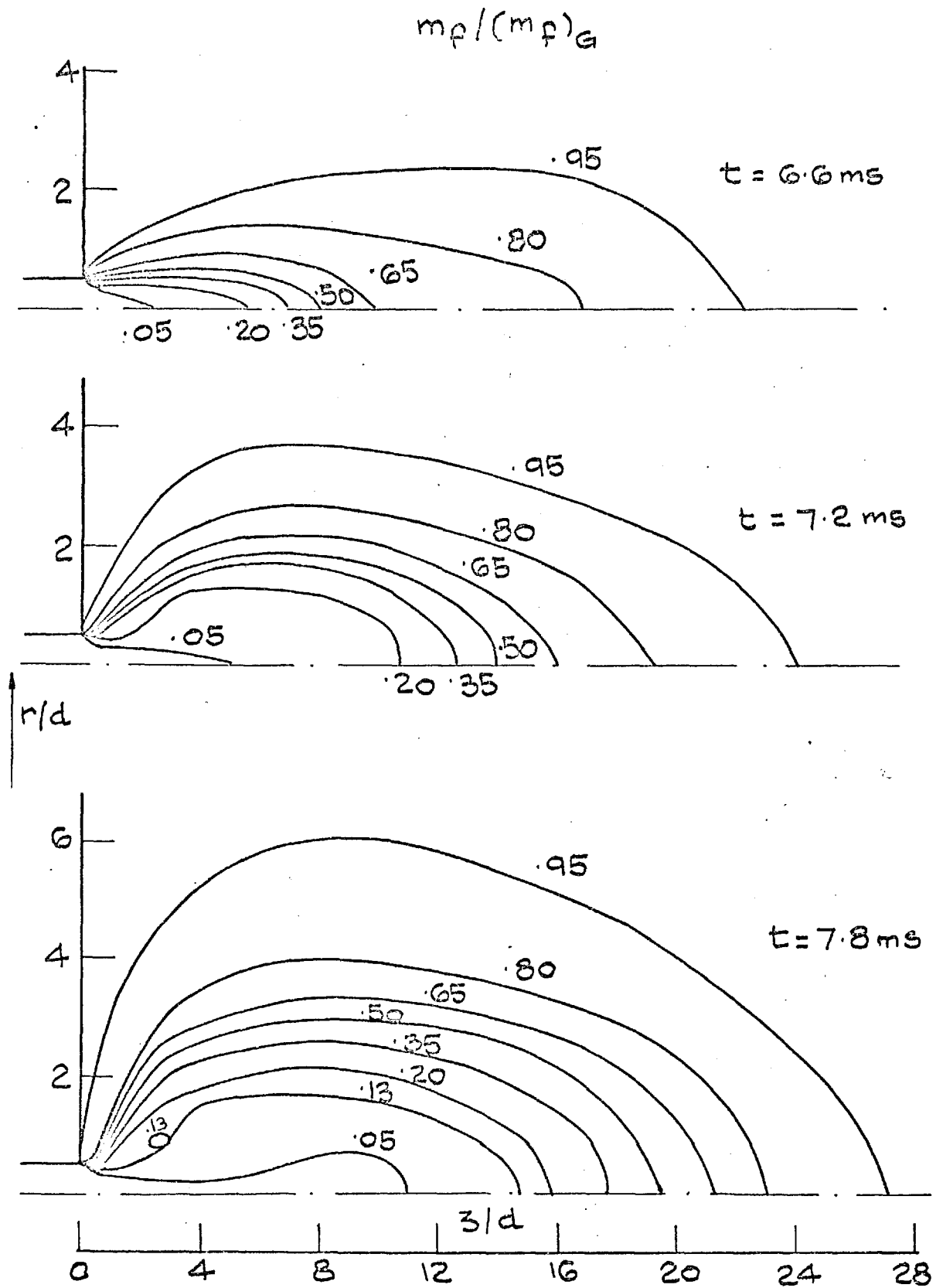


FIG. 3.6-32: DISTRIBUTION OF FUEL CONCENTRATION
AT THREE DIFFERENT TIME -
INTERVALS WITH IGNITION.

VELOCITY VECTOR (m/s)

2 m/s

SCALE:

50 m/s

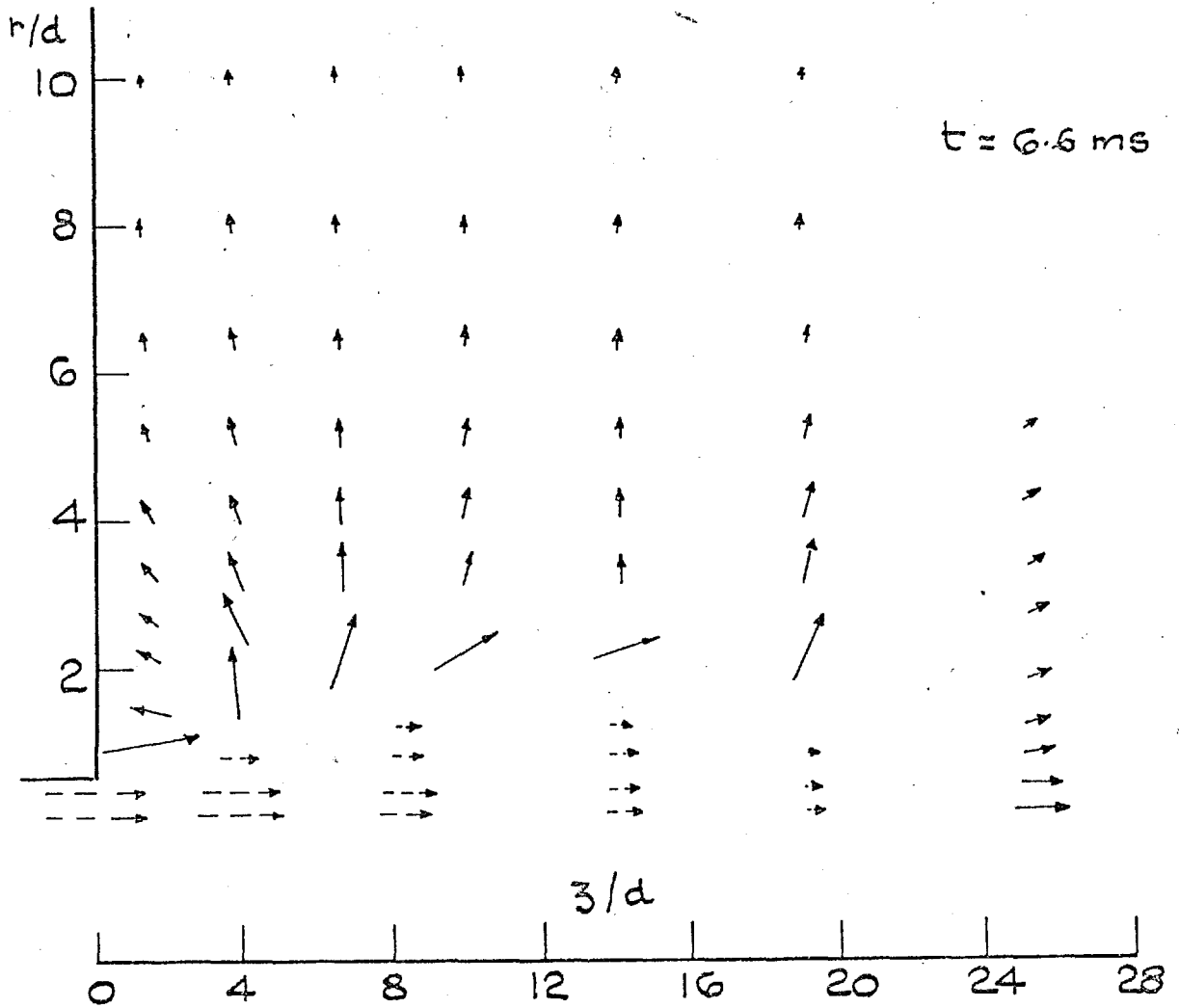


FIG. 3.6-33: VELOCITY- VECTOR DISTRIBUTION
AT $t = 6.6 \text{ ms}$ WITH IGNITION.

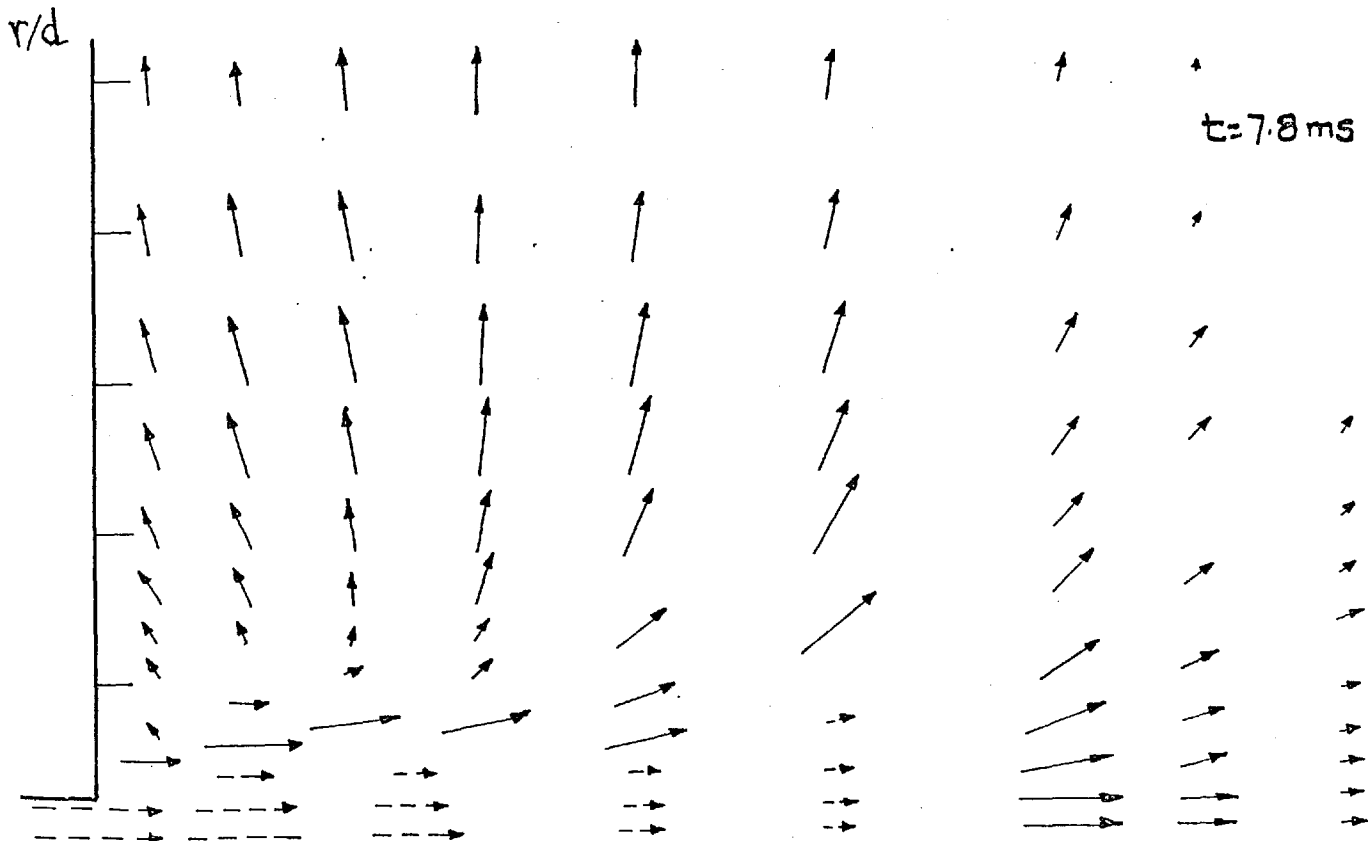
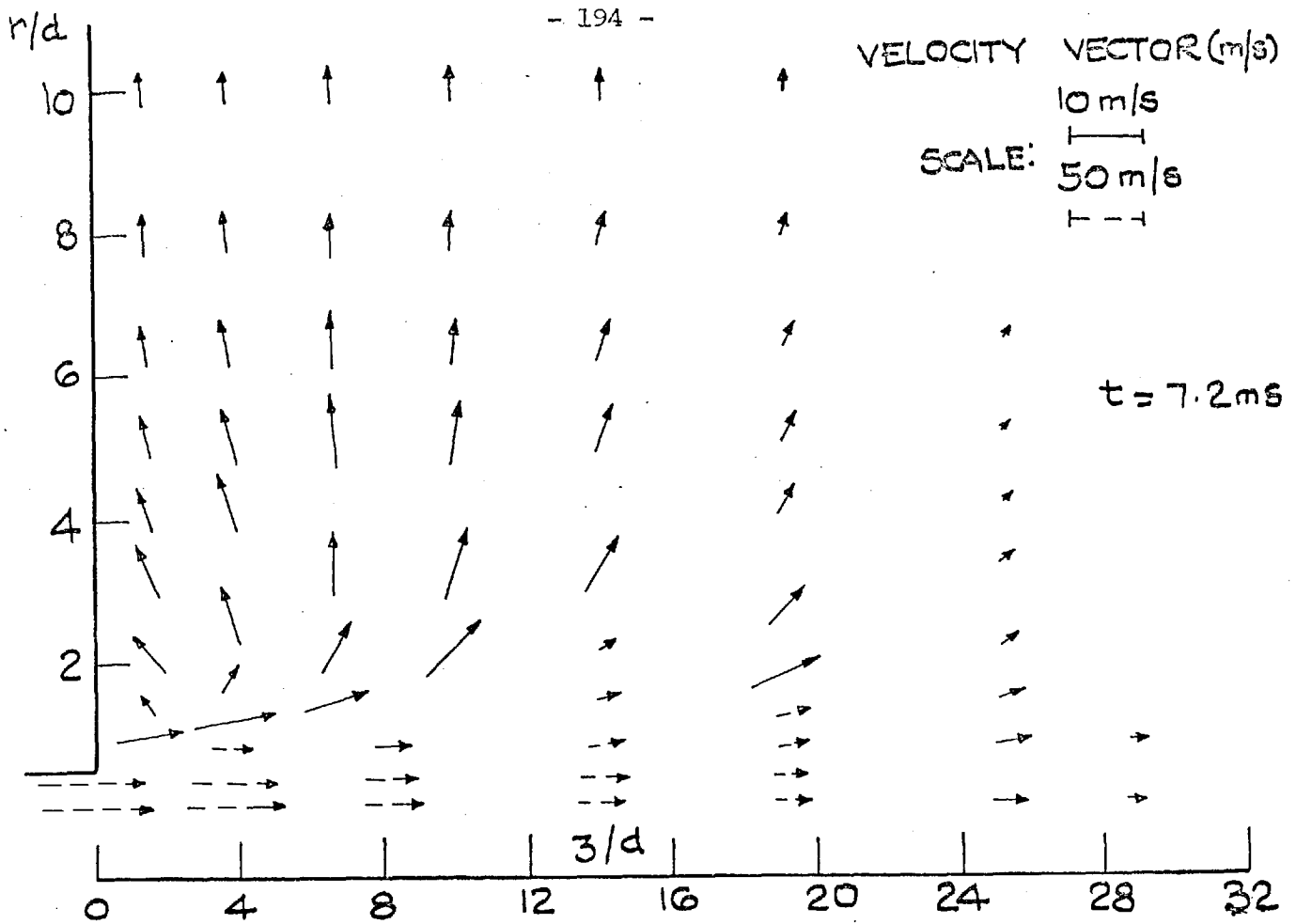


FIG. 3.6-34: VELOCITY - VECTOR DISTRIBUTION AT TWO DIFFERENT TIME - INTERVALS WITH IGNITION.

- 195 -
 $(P - P_{atm}) \text{ (N/m}^2\text{)}$

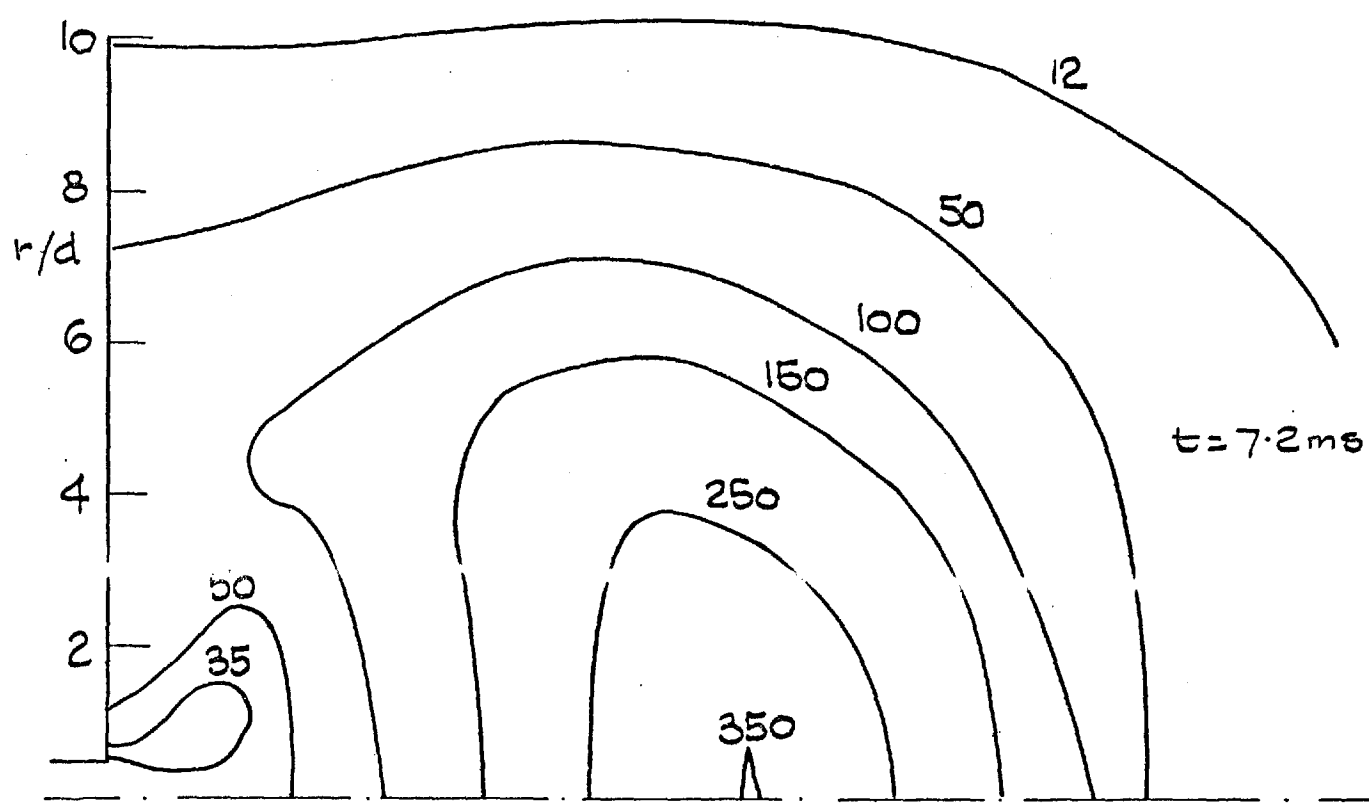
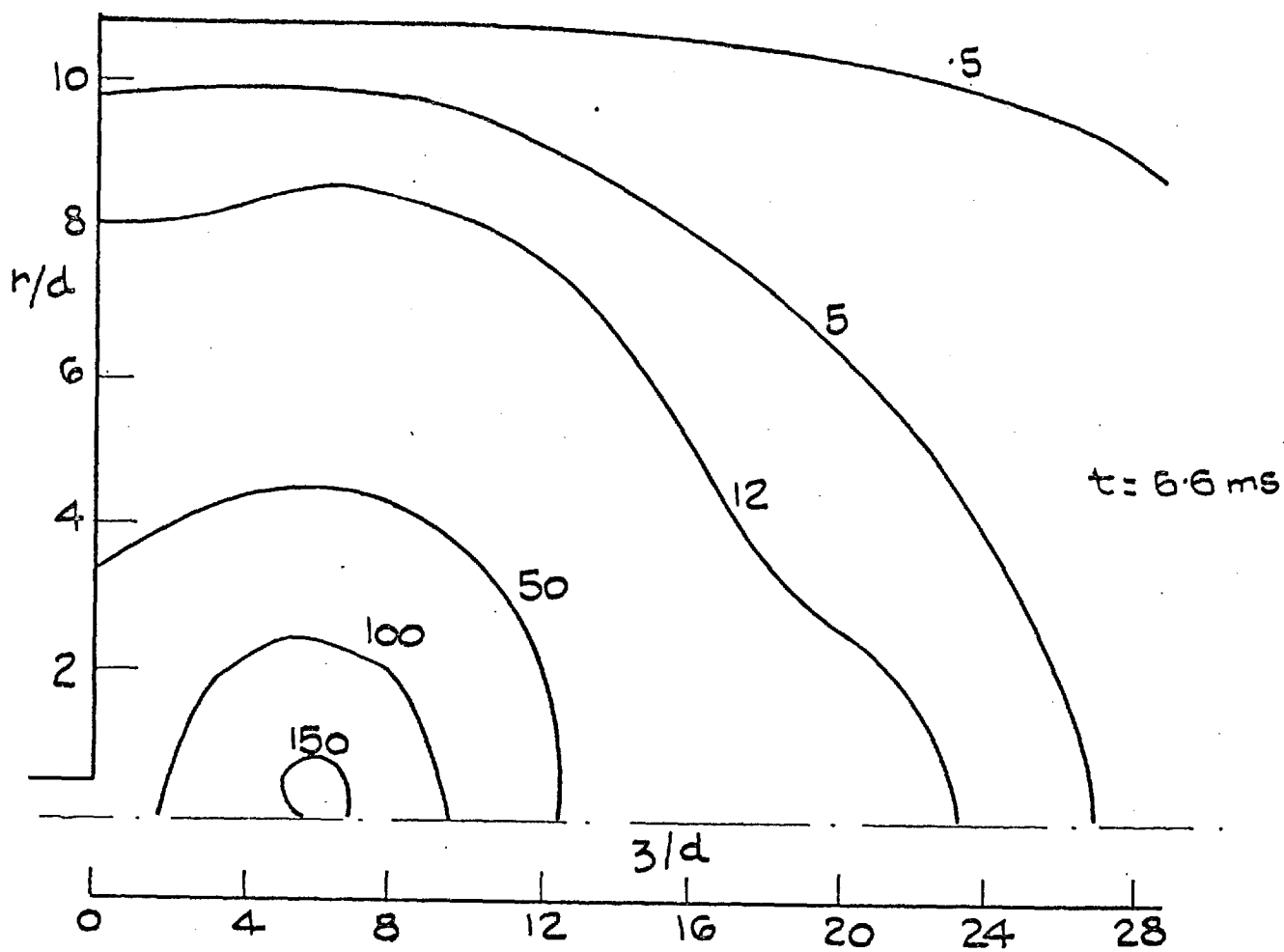


FIG. 3.6-35: STATIC PRESSURE DISTRIBUTION AT TWO DIFFERENT TIME INTERVALS WITH IGNITION.

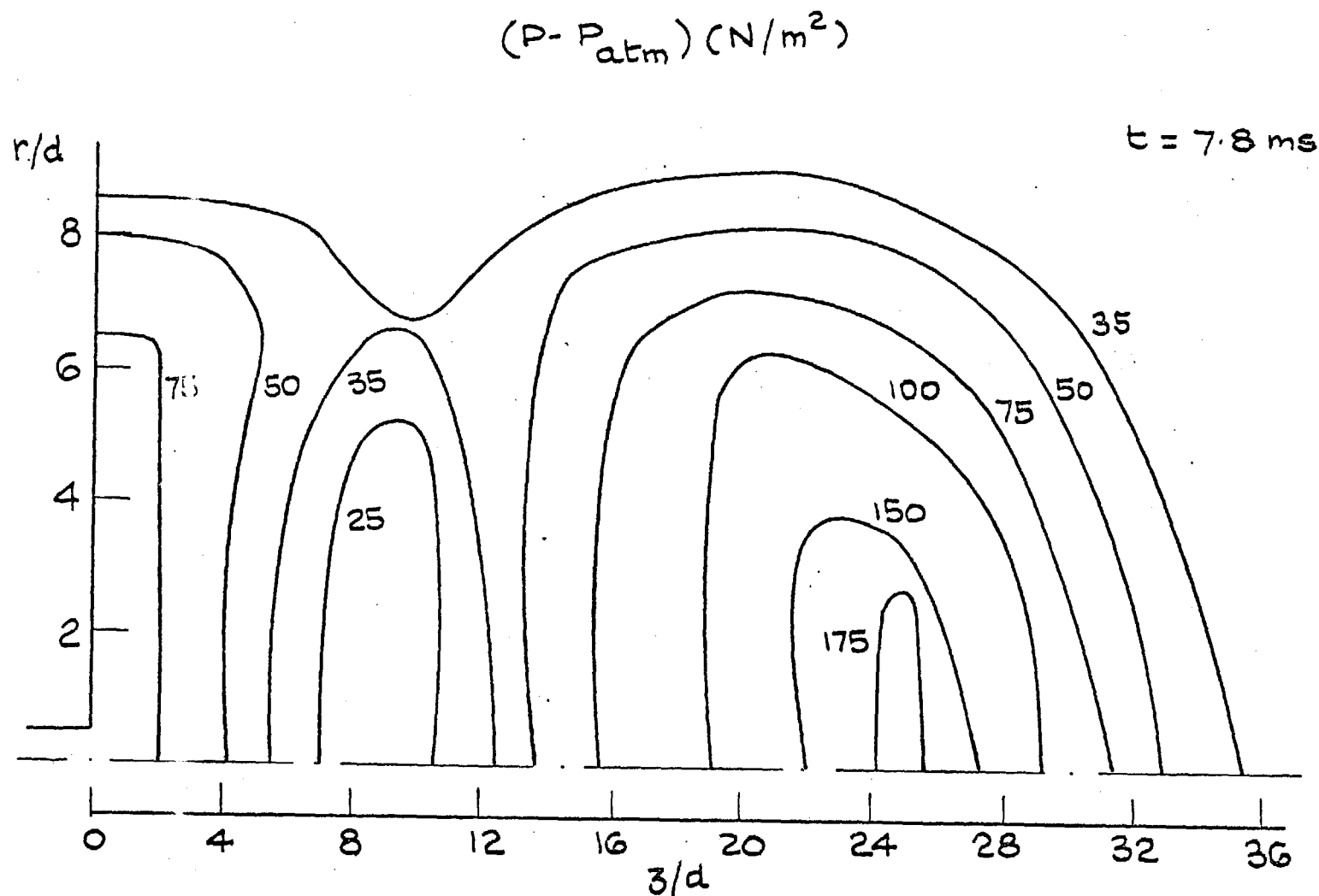


FIG. 3.6-36: STATIC PRESSURE DISTRIBUTION AT $t = 7.8 \text{ ms}$ WITH IGNITION.

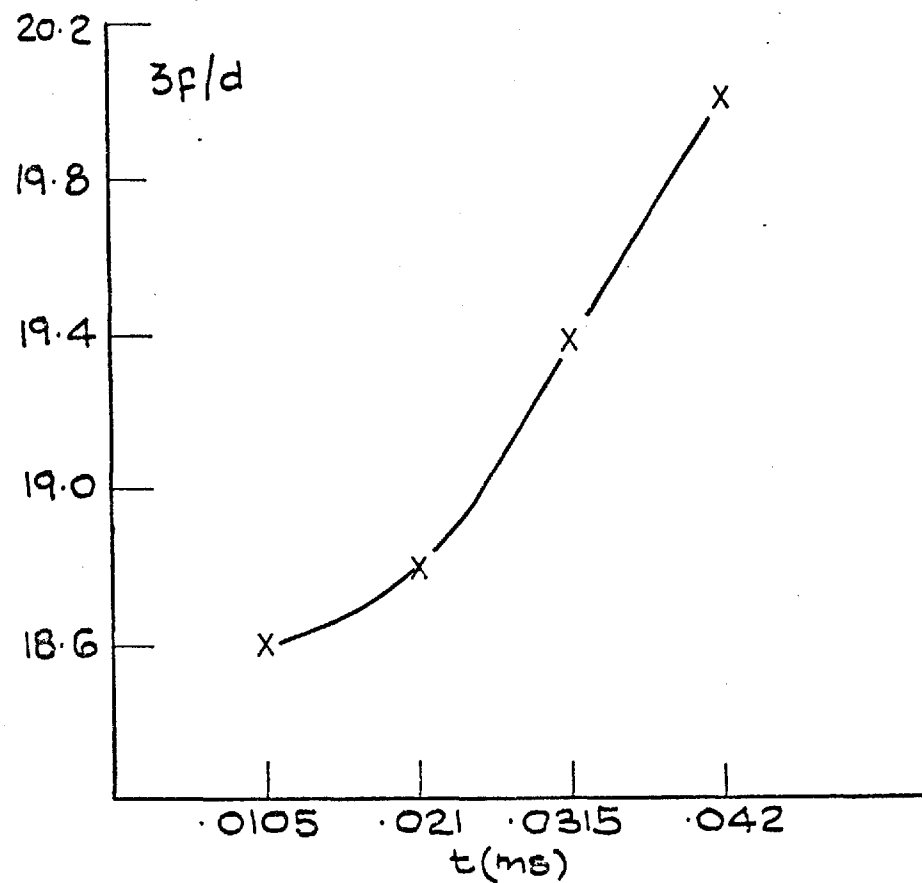


FIG. 3.6-37: EFFECT OF TIME STEP-
SIZE ON PREDICTED
JET- FRONT AT $t=10$ ms

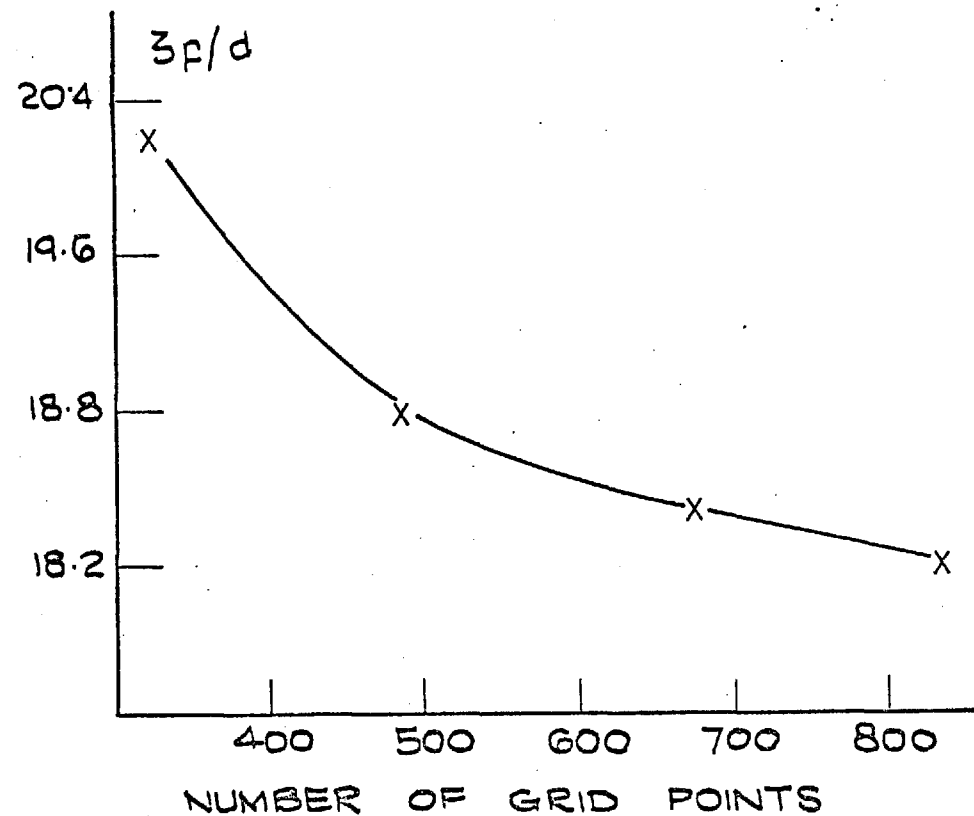


FIG. 3.6-38: EFFECT OF NUMBER OF
GRID POINTS ON PREDICTED
JET- FRONT AT $t=10$ ms.

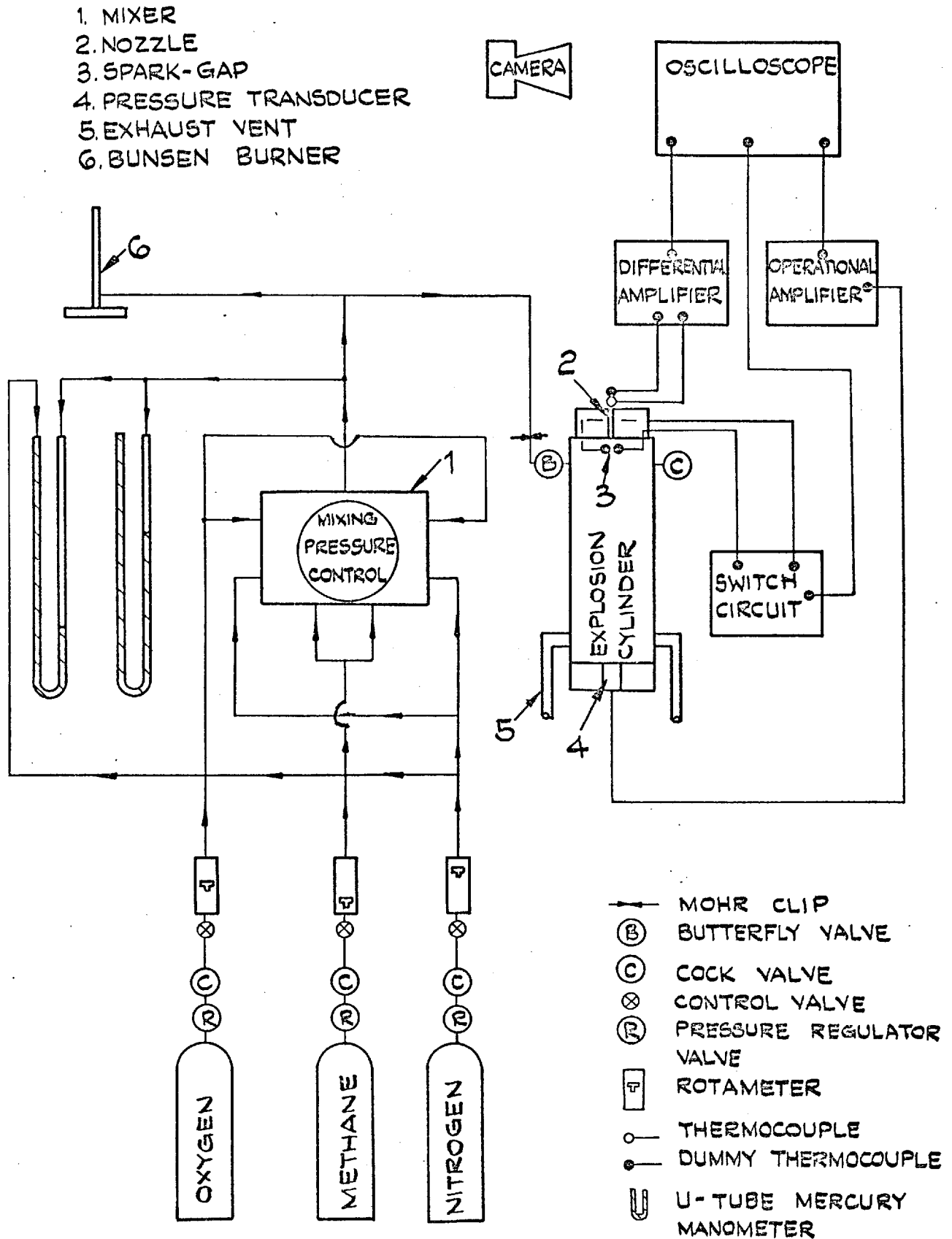


FIG. 4. 2-1: SCHEMATIC LAYOUT OF THE APPARATUS.

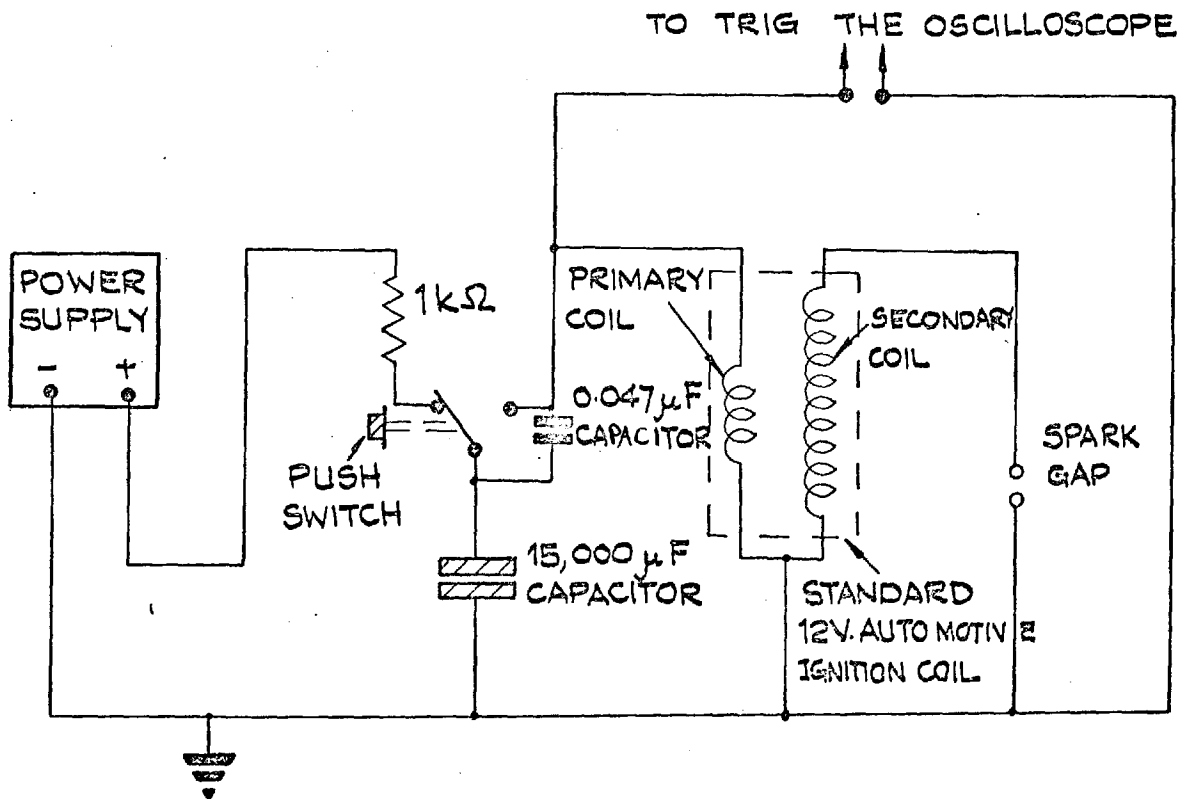


FIG. 4.2-2: ESSENTIAL FEATURES OF THE SWITCH CIRCUIT

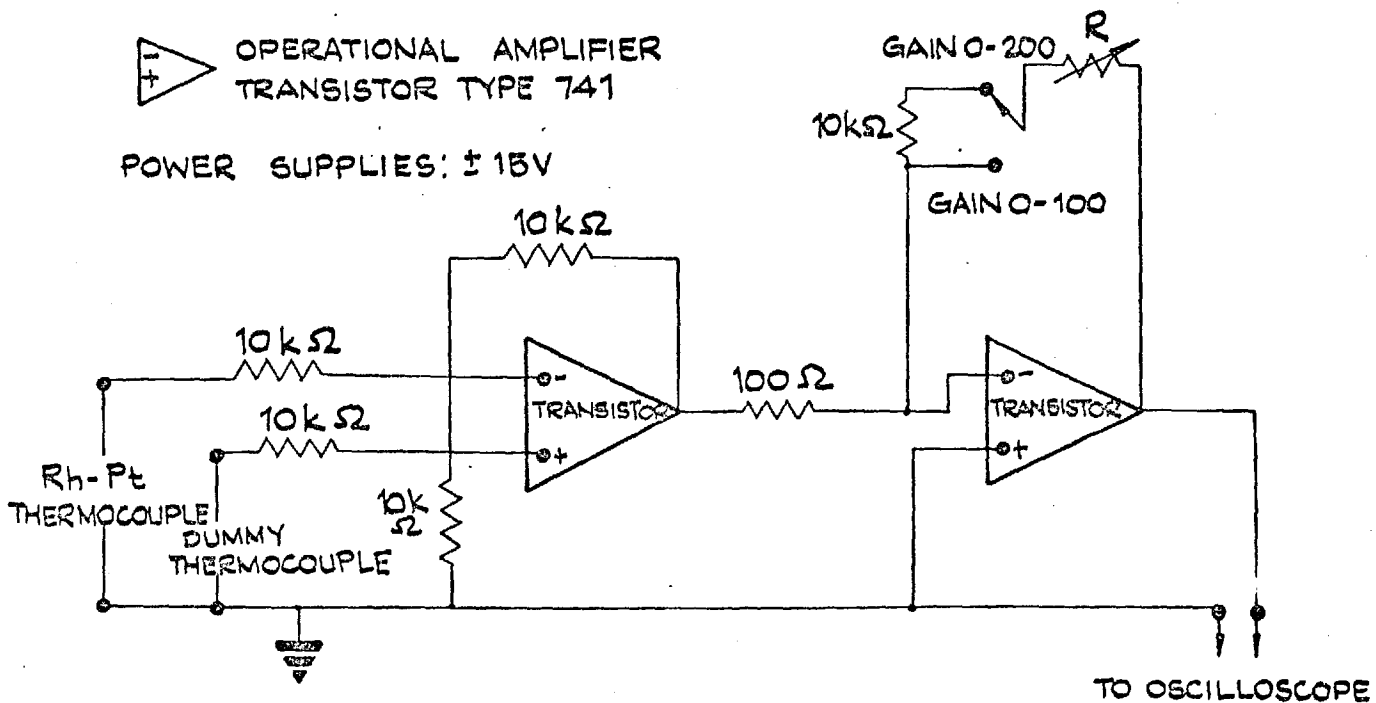


FIG. 4.2-3: DIFFERENTIAL AMPLIFIER CIRCUIT.

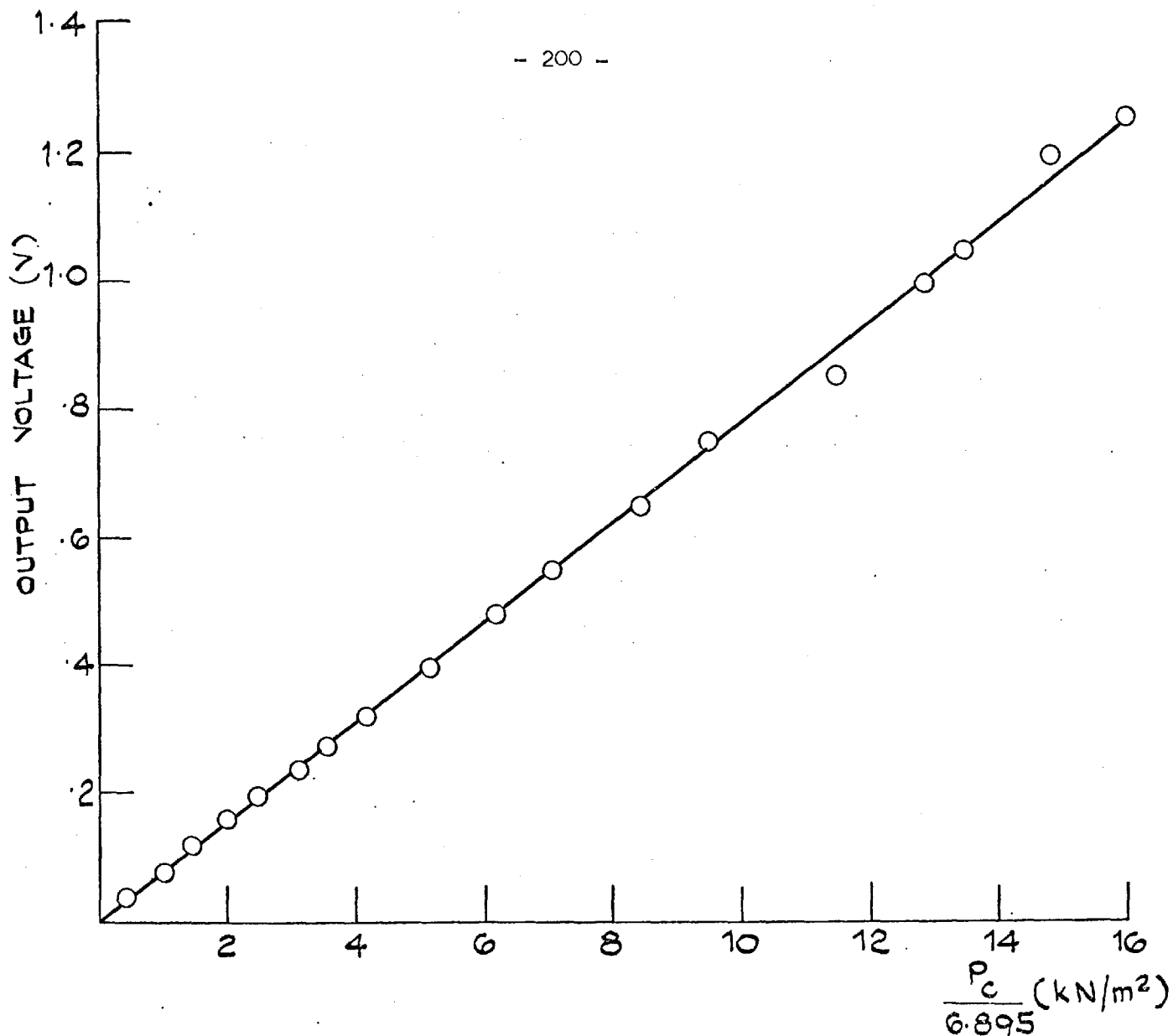


FIG. 4.3-1: CALIBRATION CURVE OF THE PRESSURE TRANSDUCER.

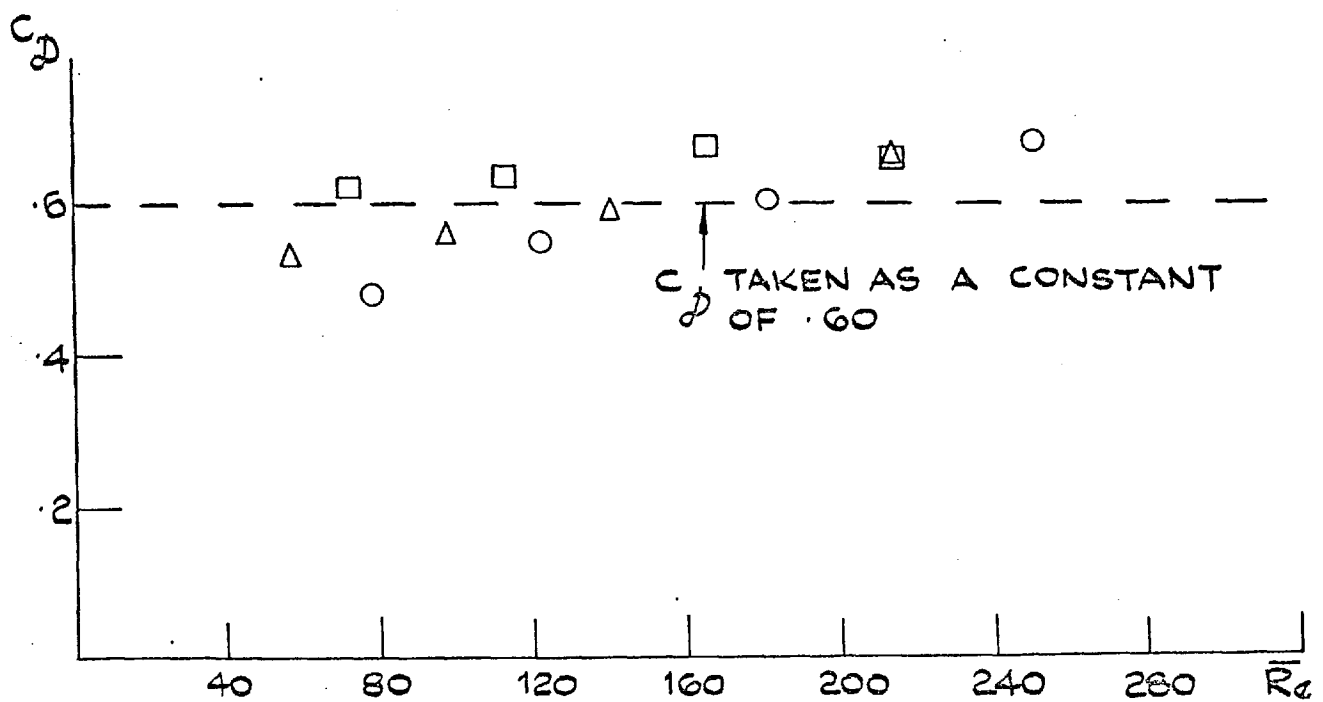


FIG. 4.3-2: VARIATION OF COEFFICIENT OF DISCHARGE WITH REYNOLDS NUMBER.

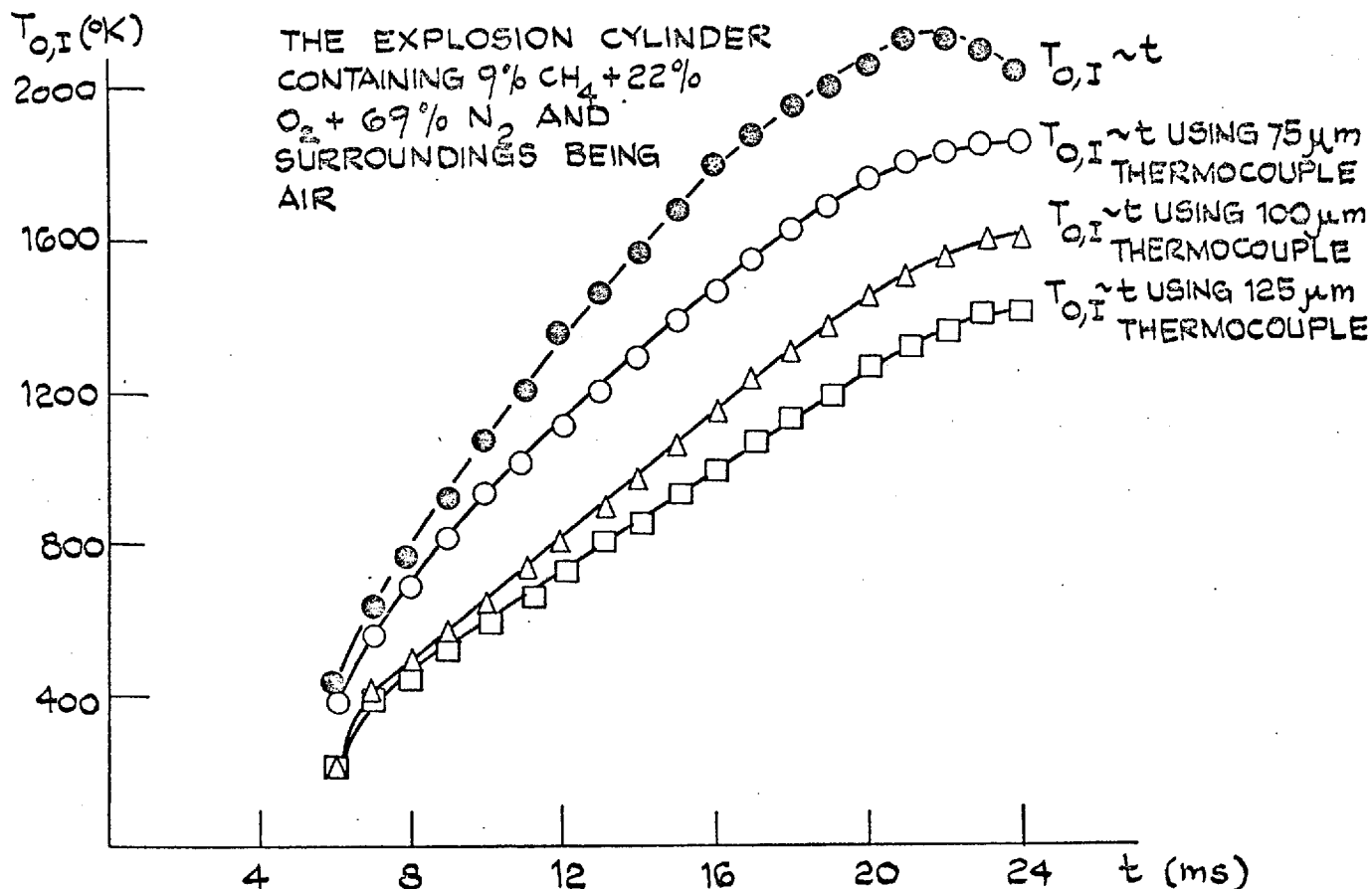


FIG. 4.4-1: DEVELOPMENT OF TEMPERATURE AT THE NOZZLE EXIT.

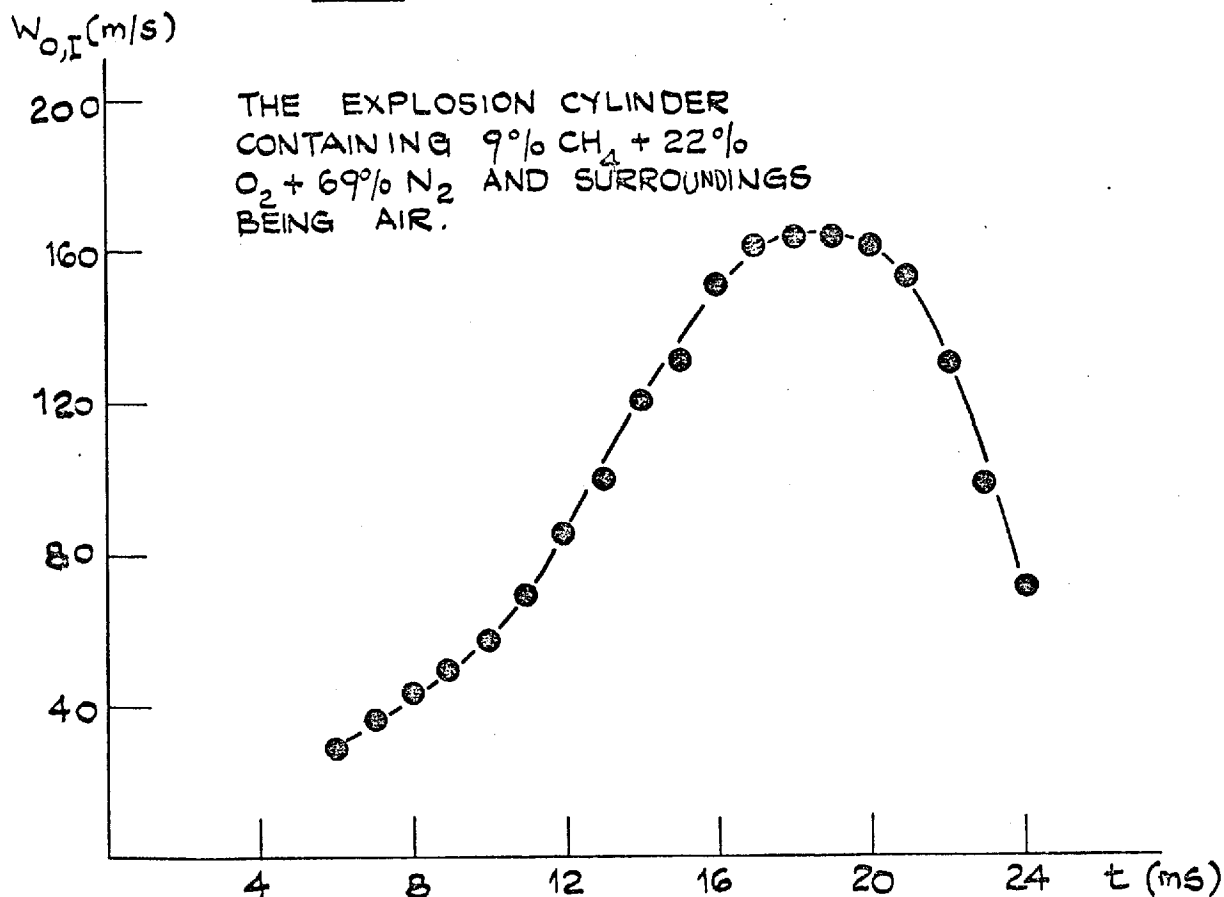


FIG. 4.6-1: DEVELOPMENT OF LONGITUDINAL VELOCITY AT THE NOZZLE EXIT.

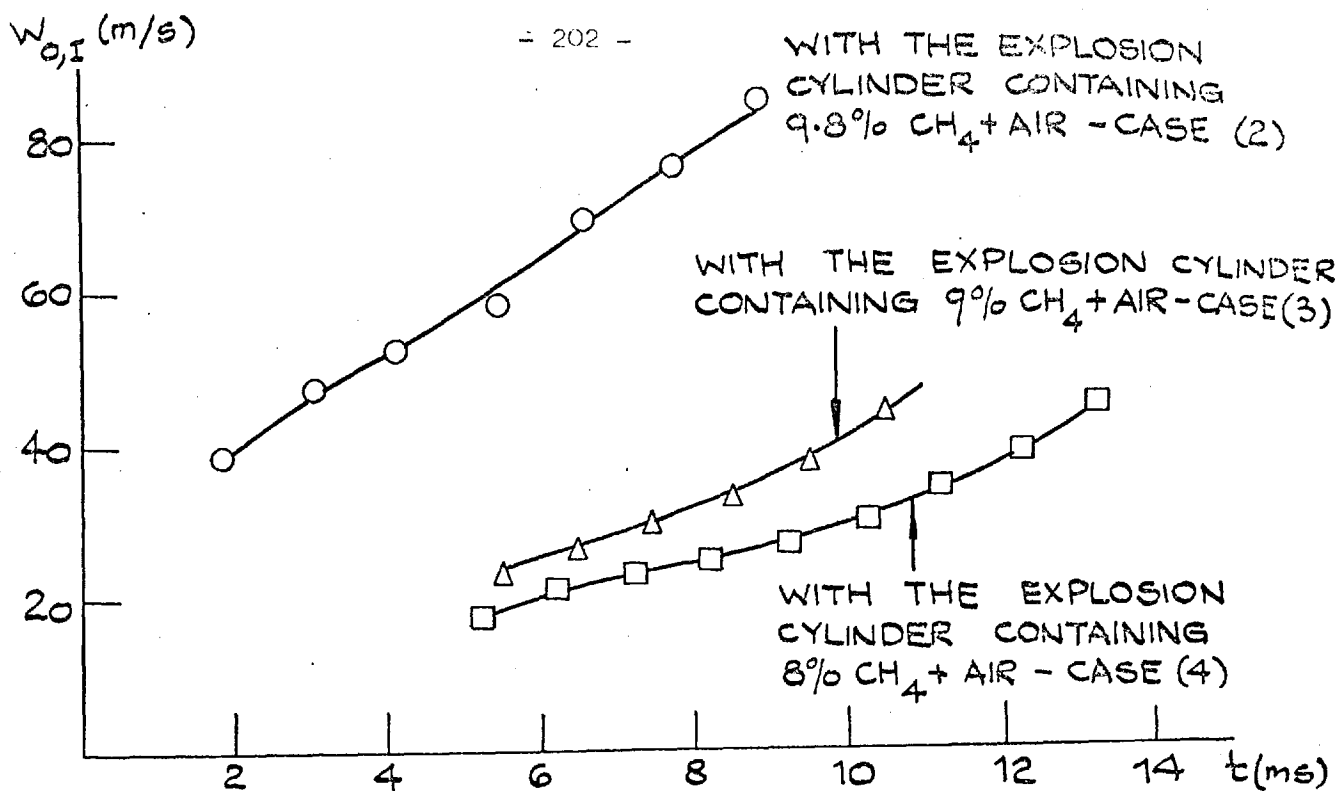


FIG. 4.6-2: DEVELOPMENTS OF LONGITUDINAL VELOCITY AT THE NOZZLE EXIT.

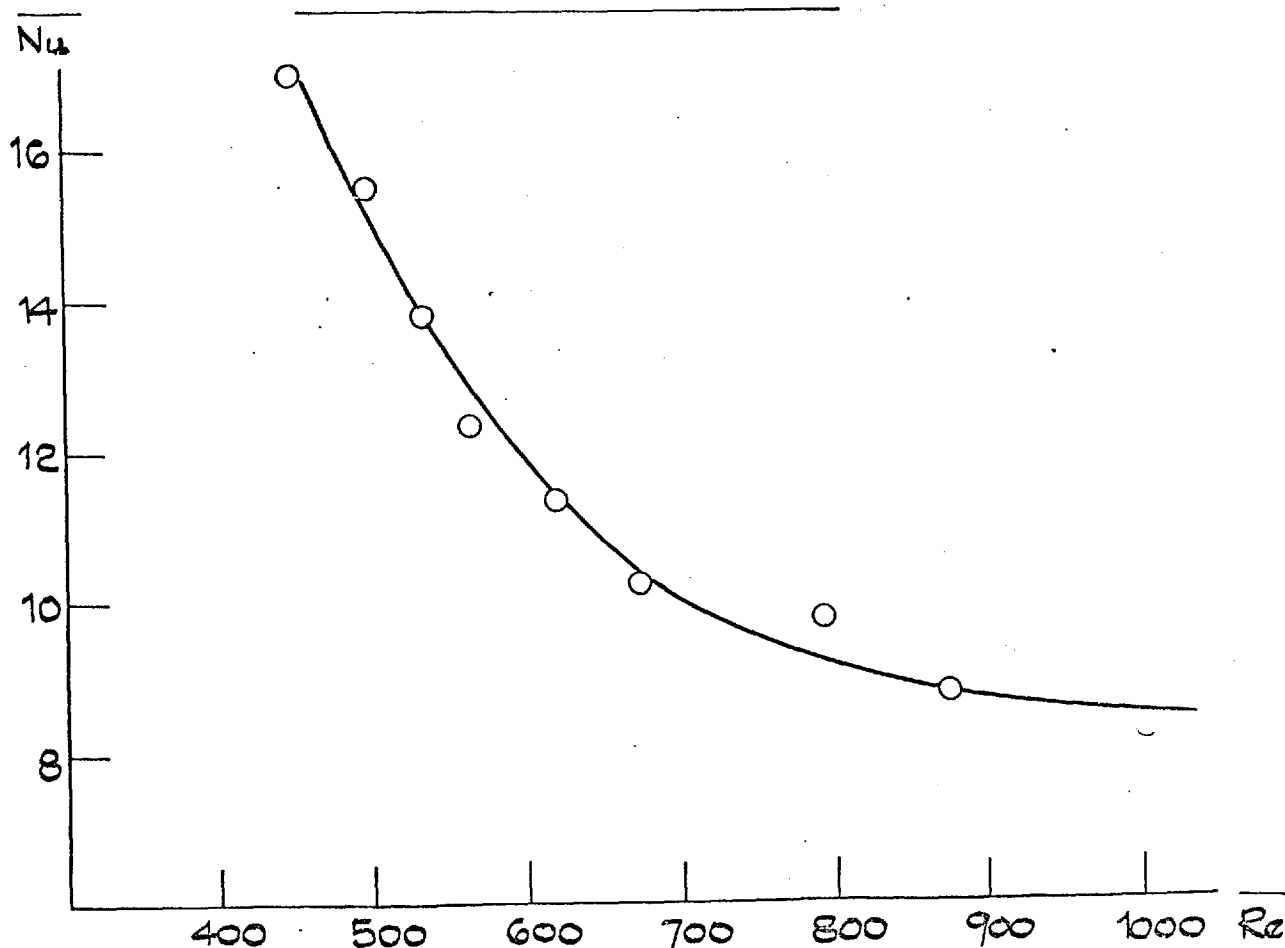


FIG. 4.6-3: VARIATION OF NUSSELT NUMBER WITH REYNOLDS NUMBER FOR A FLOW OF HOT GASES THROUGH THE NOZZLE PASSAGE.

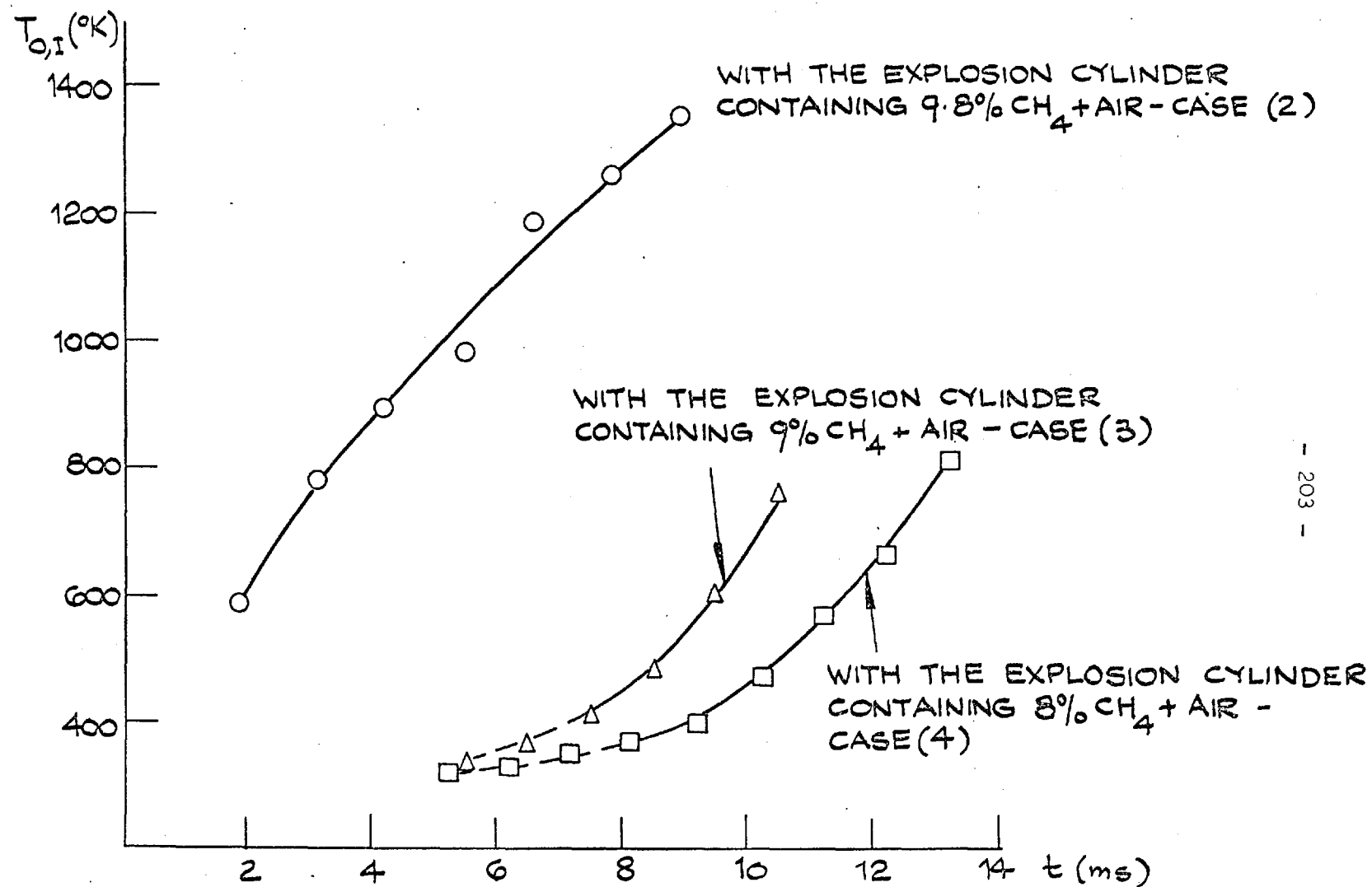


FIG. 4.6-4: DEVELOPMENTS OF TEMPERATURE AT THE NOZZLE EXIT.

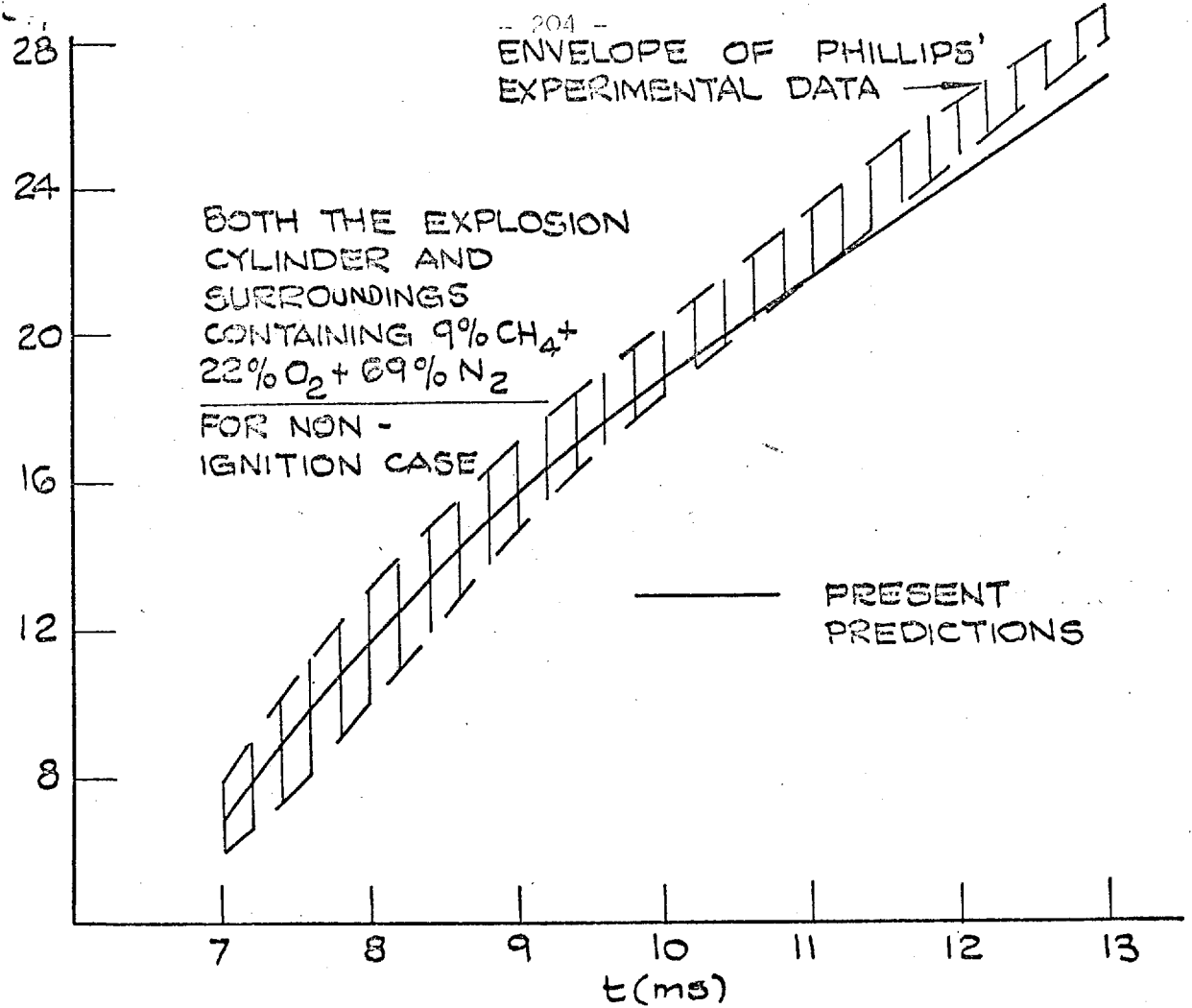


FIG. 5.2-1: COMPARISON OF THE PREDICTED AND EXPERIMENTAL DEVELOPMENTS OF JET-FRONT.

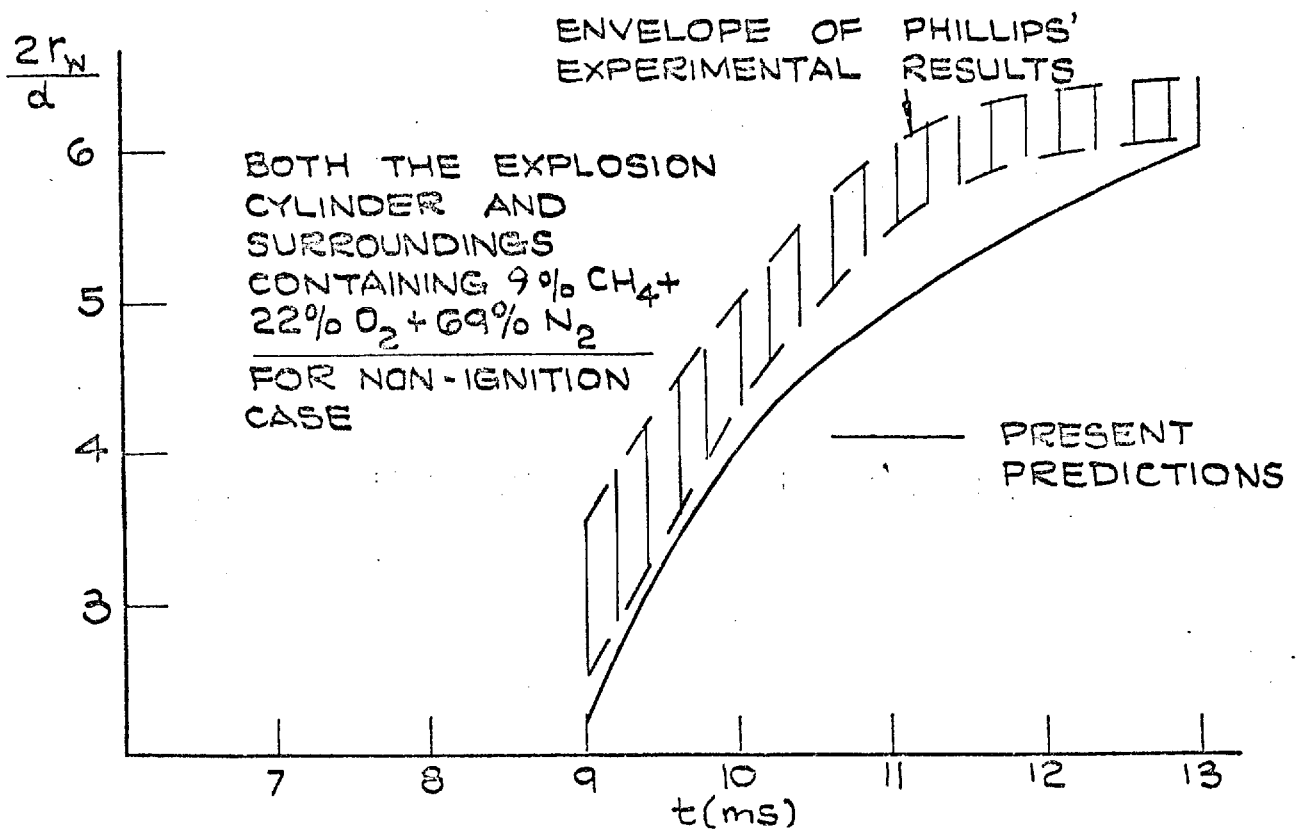


FIG. 5.2-2: COMPARISON OF THE PREDICTED AND EXPERIMENTAL DEVELOPMENT OF JET-WIDTH AT $z/d = 16.25$.

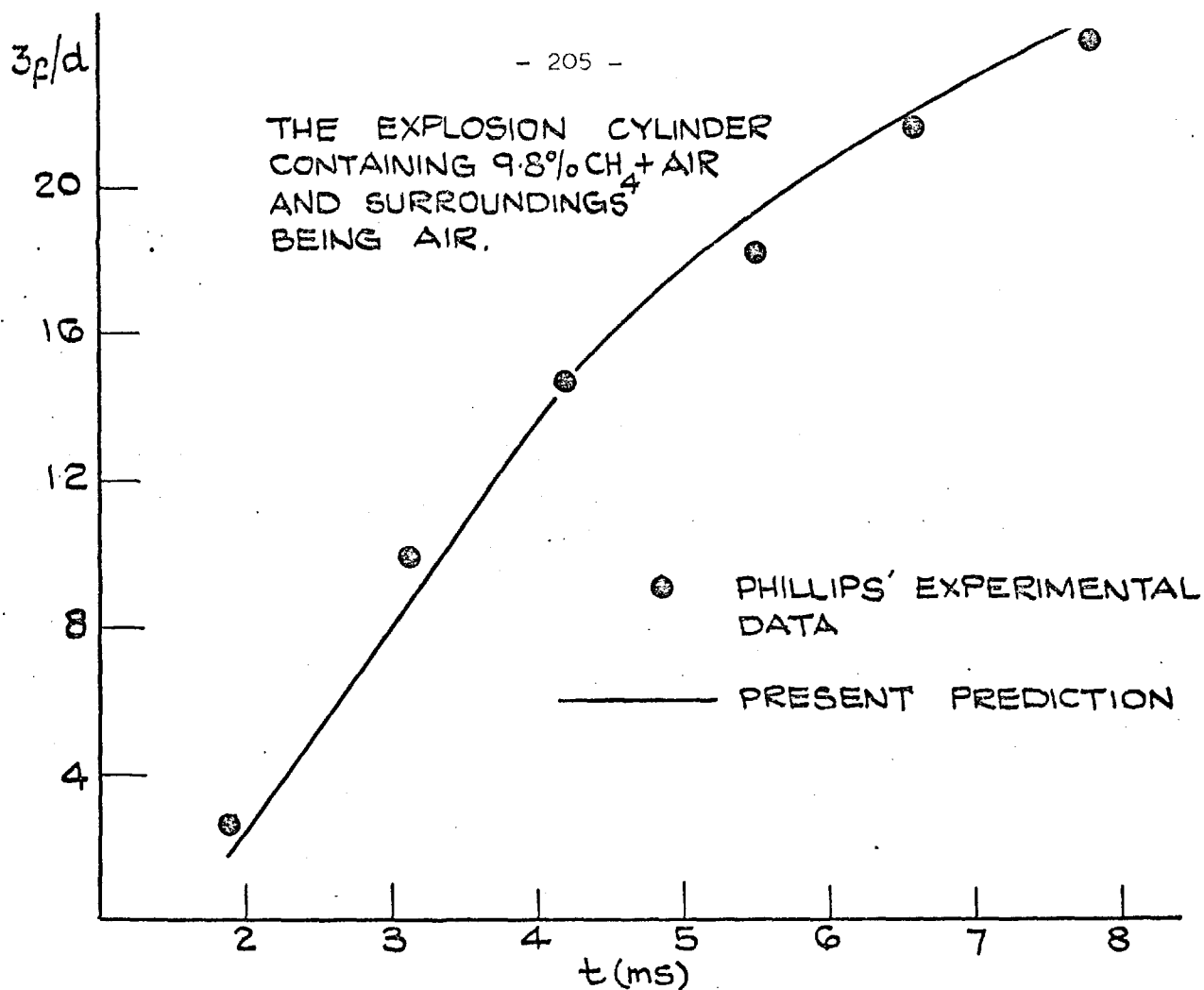


FIG. 5.2-3: COMPARISON OF THE PREDICTED AND EXPERIMENTAL DEVELOPMENTS OF JET-FRONT.

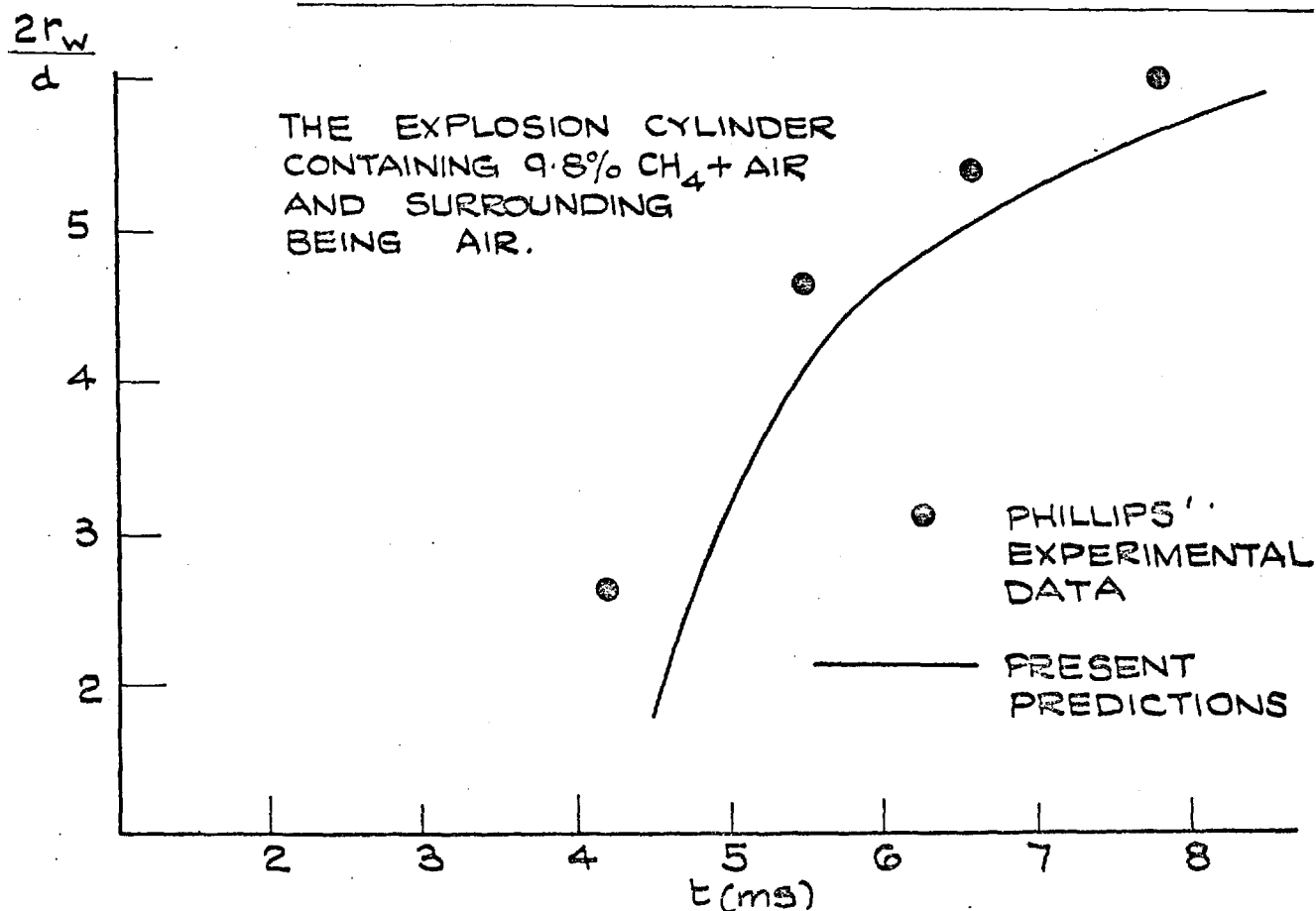


FIG. 5.2-4: COMPARISON OF PREDICTED AND EXPERIMENTAL DEVELOPMENTS OF JET-WIDTH AT $3/d = 14.25$.

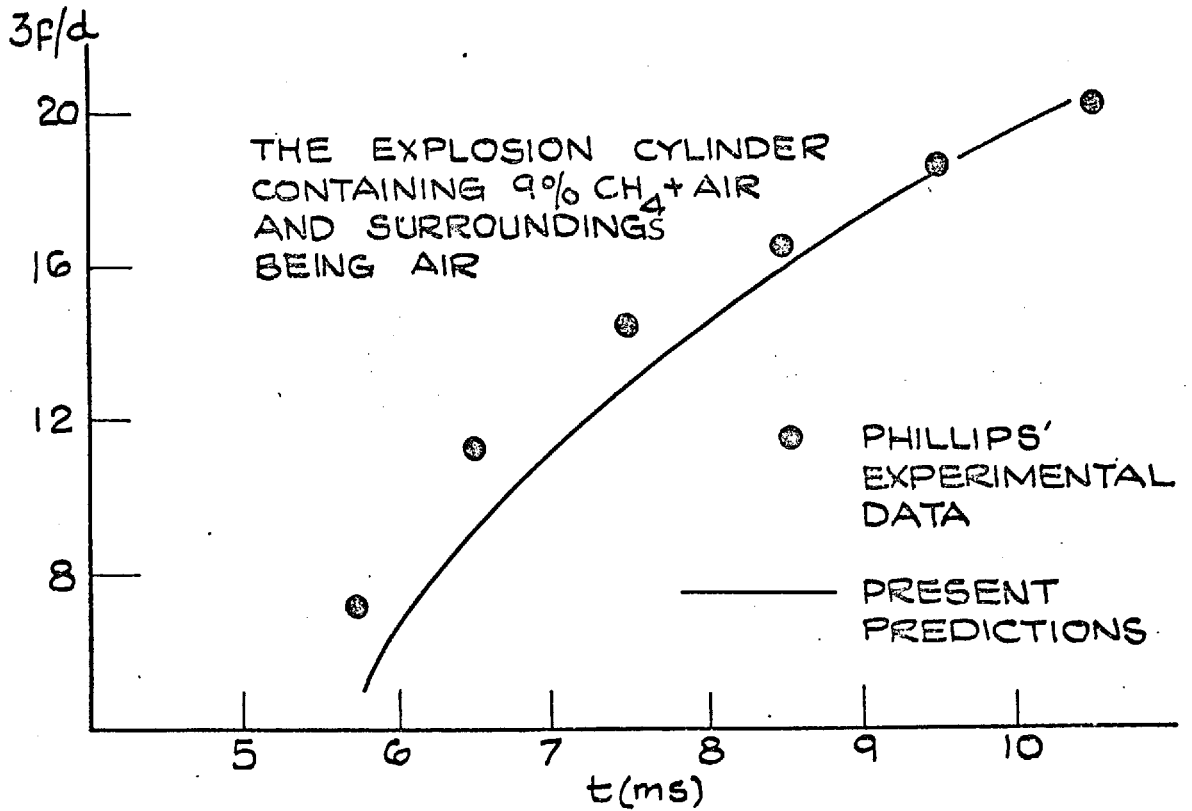


FIG. 5.2-5 : COMPARISON OF THE PREDICTED AND EXPERIMENTAL DEVELOPMENTS OF JET-FRONT.

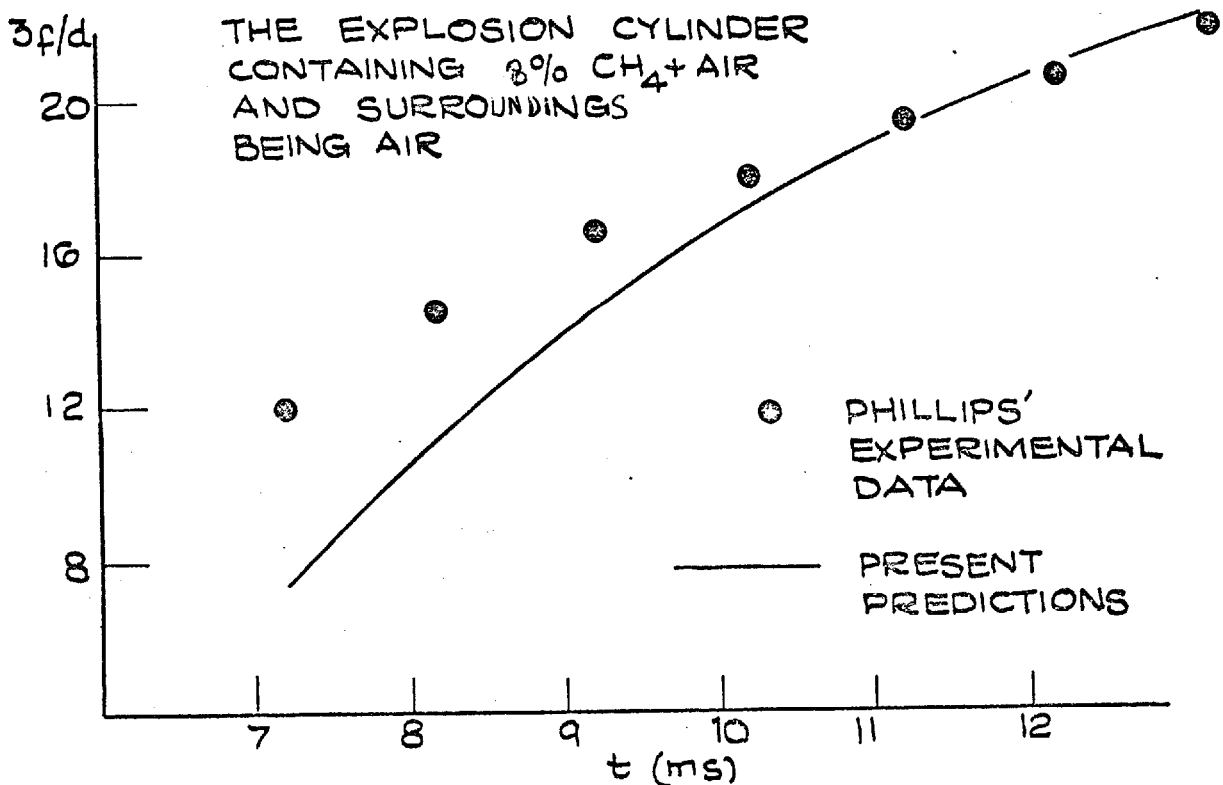


FIG. 5.2-6 : COMPARISON OF THE PREDICTED AND EXPERIMENTAL DEVELOPMENTS OF JET-FRONT.

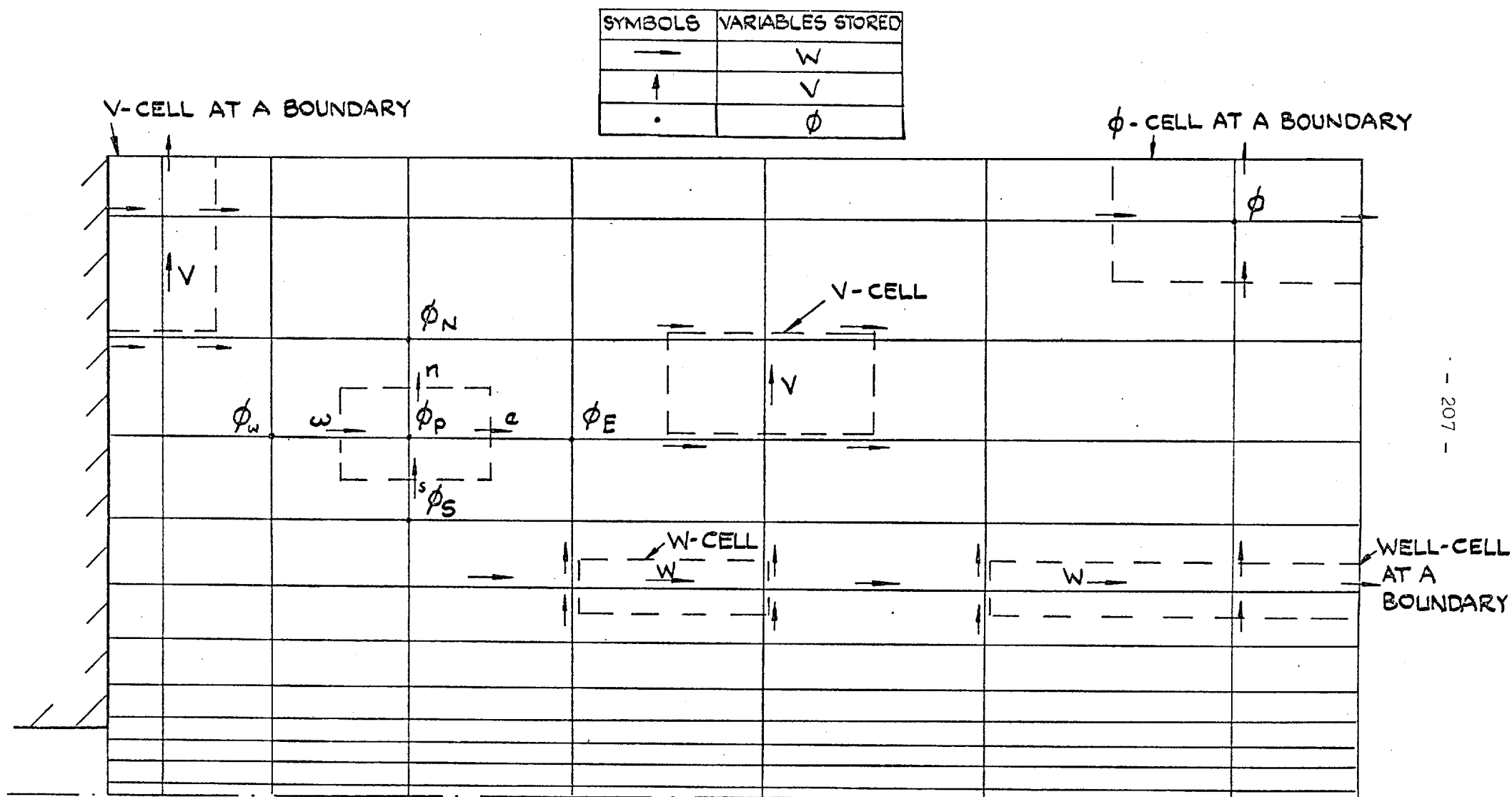


FIG. B.1: CONTROL-VOLUME ARRANGEMENTS FOR EACH OF THE DEPENDENT VARIABLES.

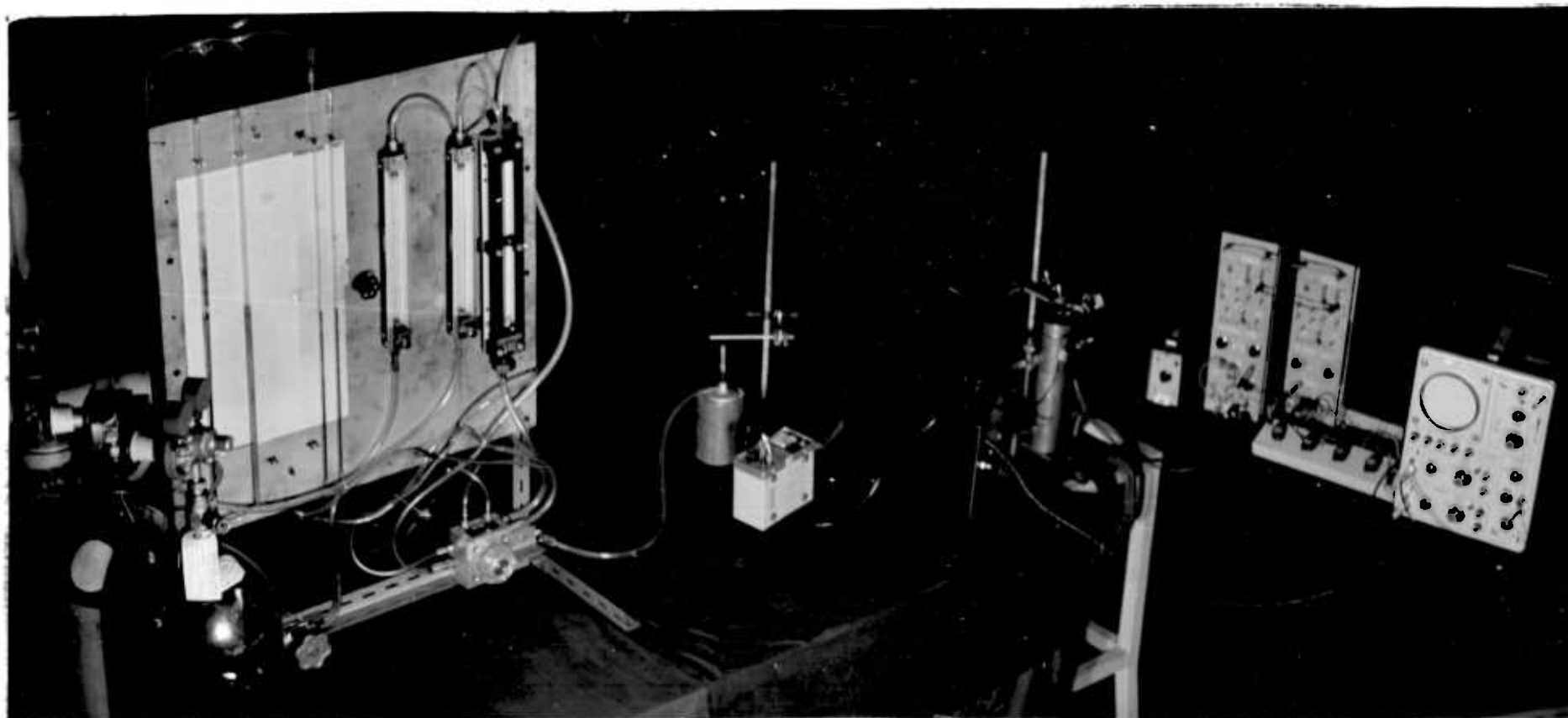


Plate I: Arrangement of experimental apparatus

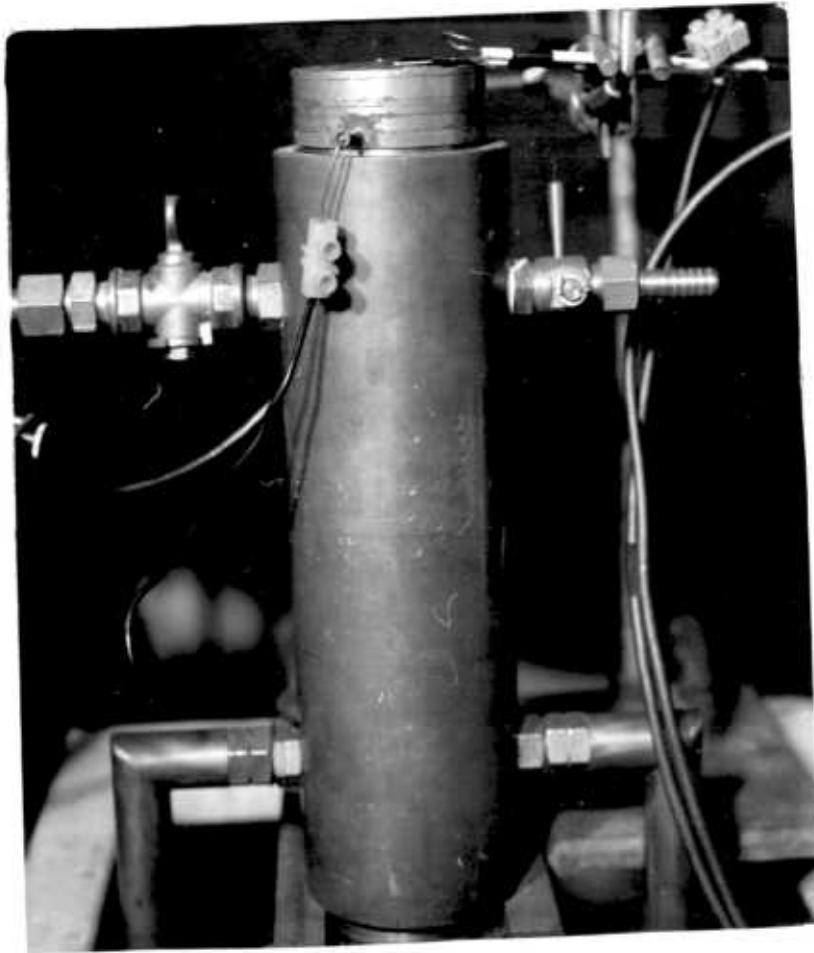


Plate III: Front view of the explosion cylinder

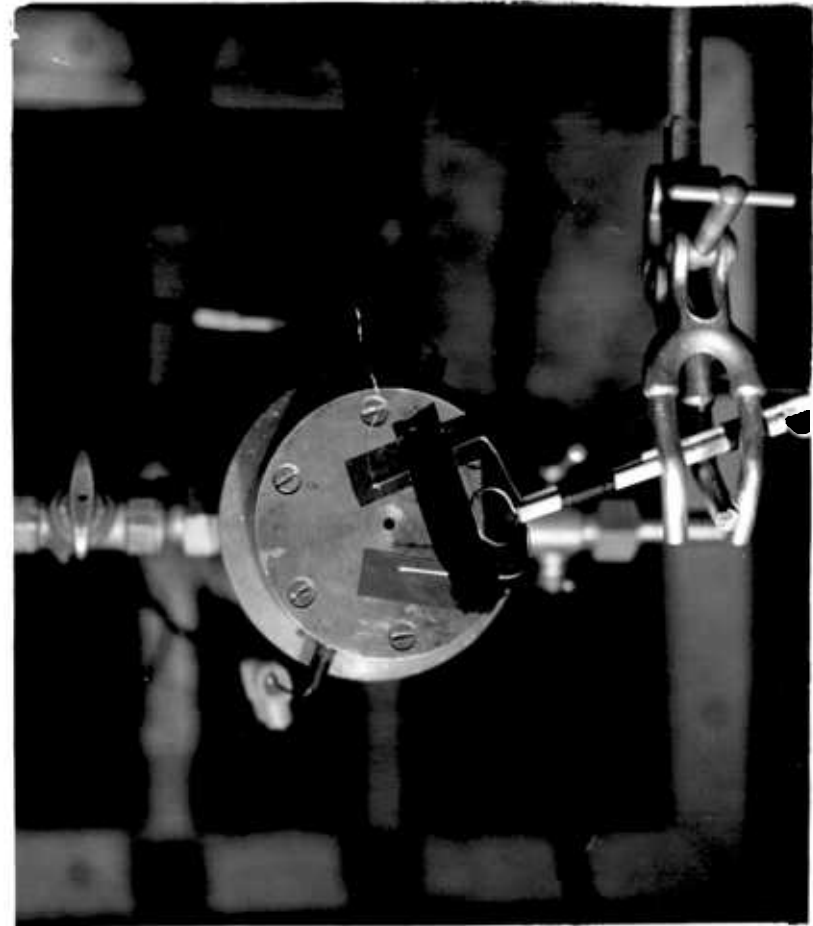


Plate II: Top view of the explosion cylinder and thermocouple probe in measuring position

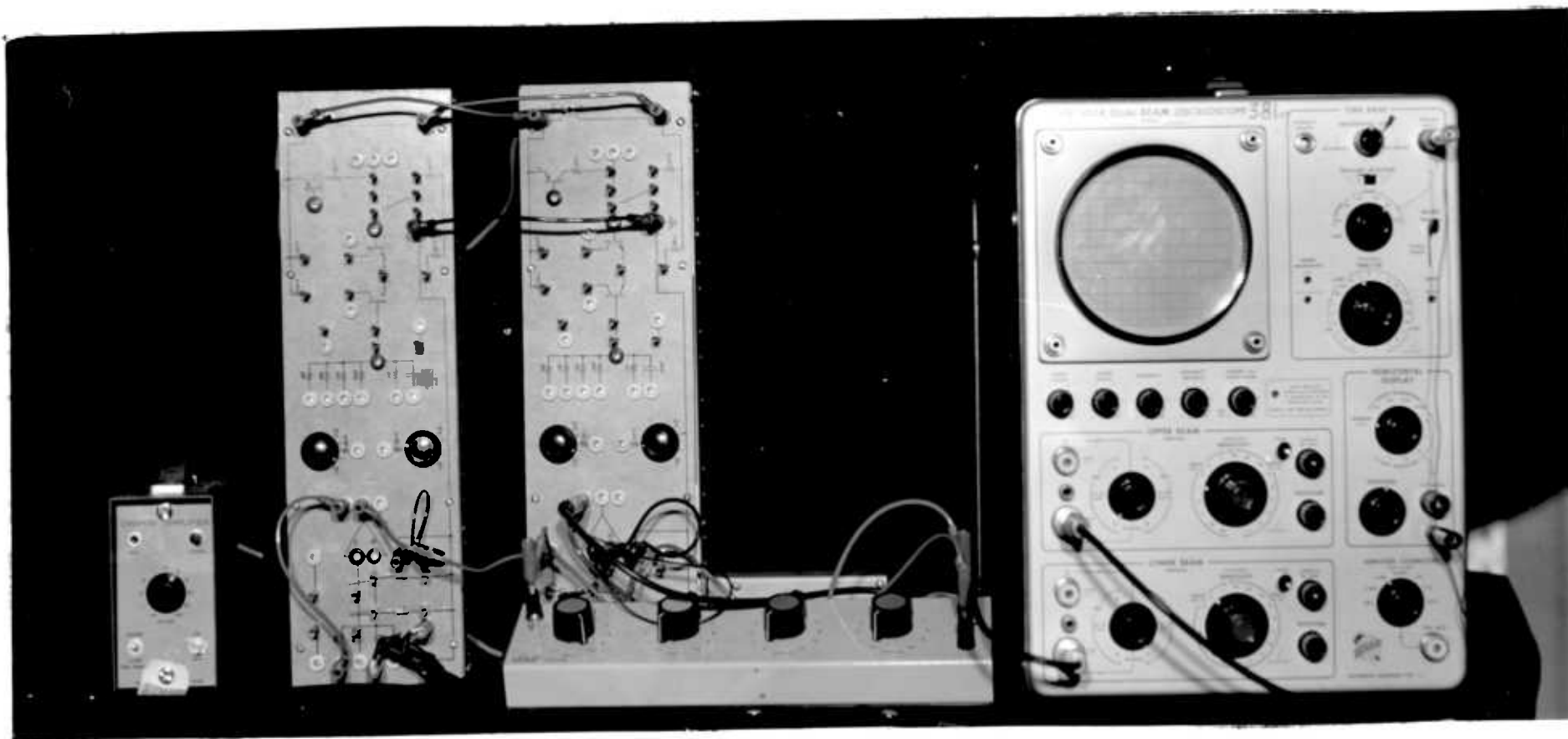


Plate IV: The charge amplifier, the differential amplifier and the oscilloscope

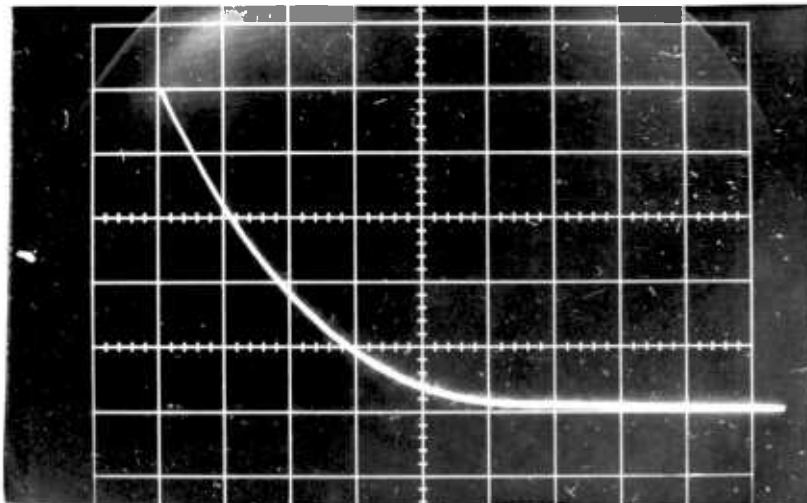


Plate V: Oscilloscope trace displaying the decrease with
time of pressure inside the explosion cylinder
in the 'cold' flow test

<u>Scale</u>	Horizontal	-	1 cm	:	5 ms
	Vertical	-	1 cm	:	.1 V.

Plate VI: Developments of temperature at the nozzle exit (with 75 μ m thermocouple) and pressure inside the explosion cylinder

Scale

Horizontal - 1 cm : 5 ms

Vertical - 1 cm : 1 mv (temperature curve)

1 cm : .2 V (pressure curve)



Plate VII: Developments of temperature at the nozzle exit (with 100 μ m thermocouple) and pressure inside the explosion cylinder

Scale

Horizontal - 1 cm : 5 ms

Vertical - 1 cm : .5 mv (temperature curve)

1 cm : .2 V (pressure curve)



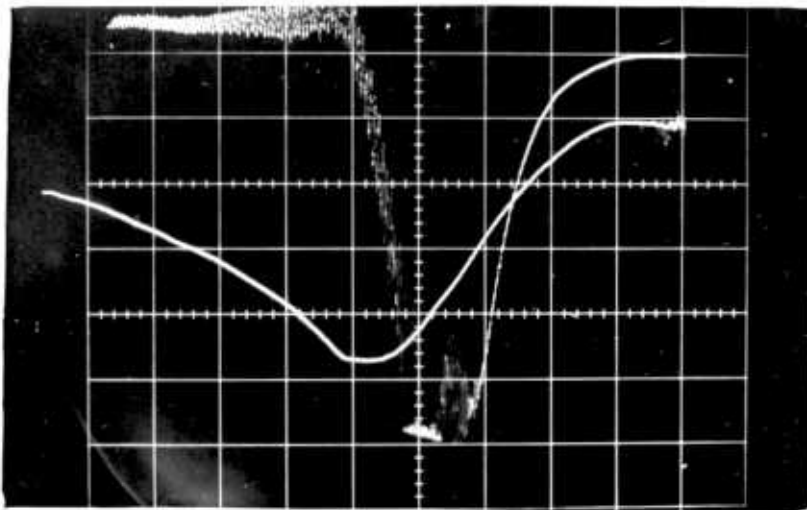
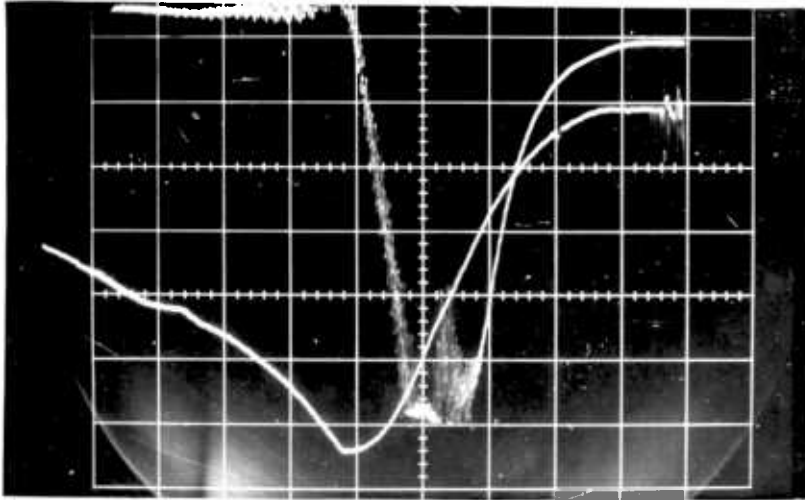


Plate VIII: Development of temperature at the nozzle exit
(with 125 μ m thermocouple) and pressure inside
the explosion cylinder

Scale

Horizontal - 1 cm : 5 ms

Vertical - 1 cm : 1 mv (temperature curve)

1 cm : .2 V. (pressure curve)



Plate IX: The same as that in Plate VIII but with the horizontal time
scale doubled to 1 cm : 10 ms

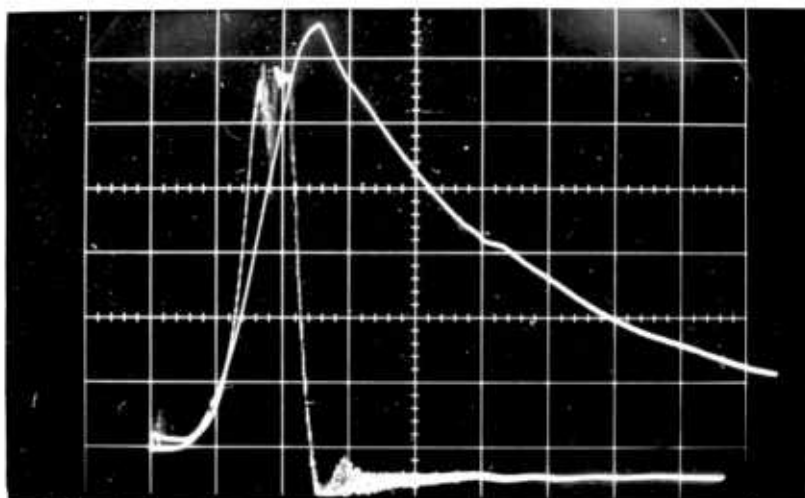
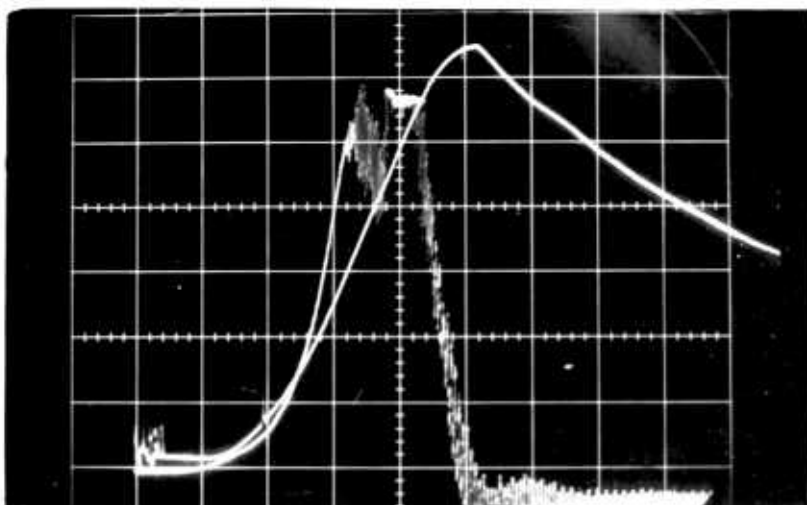


Plate X Phillips' Schlieren photographs showing the development of
starting-jets for non-ignition cases

Picture set for case no. (from top)	Prepared mixture inside the explosion cylinder	Initial mixture in the surroundings
1	9% CH ₄ + 22% O ₂ + 69% N ₂	9% CH ₄ + 22% O ₂ + 69% N ₂
2	9.8% CH ₄ + air	air
3	9% CH ₄ + air	air
4	8% CH ₄ + air	air



Case 1

15 14 13 12 11 10 9 8



Case 2

8.9 7.8 6.6 5.5 4.2 3.1 1.9



Case 3

13.5 12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5



Case 4

14.2 13.2 12.2 11.2 10.2 9.2 8.2 7.2 6.2

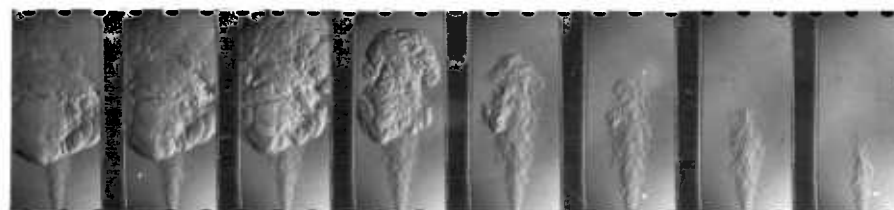
Plate XI Phillips' Schlieren photographs showing the development
of starting-jets for ignition cases

Picture set for case no. (from top)	Prepared mixture inside the explosion cylinder	Initial mixture in the surroundings
1,2,3	9% CH ₄ + 22% O ₂ + 69% N ₂	9% CH ₄ + 22% O ₂ + 69 %N ₂
4	9.8% CH ₄ + air	9.8% CH ₄ + air



Case 1

17 16 15 14 13 12 11 10 9 8 7



Case 2

15 14 13 12 11 10 9 8



Case 3

16 15 14 13 12 11 10 9



Case 4

10.0 8.9 7.8 6.6 5.5 4.2 3.1 1.0

Appendix A: Derivation of wall functions

Wall shear stress

In the vicinity of the wall, the velocity profile is given by the following universal log-law relationship:

$$\frac{V}{V_\tau} = \frac{1}{.437} \ln(8.8z^+) \quad \text{for } z^+ > 11.63 \quad (\text{A.1})$$

$$\frac{V}{V_\tau} = z^+ \quad \text{for } z^+ \leq 11.63$$

where, $V_\tau \equiv \sqrt{\frac{\tau_s}{\rho}}$ (A.2)

$$z^+ \equiv \frac{\rho z V_\tau}{\mu} = \frac{\rho z}{\mu} \frac{\tau_s}{\rho} \quad (\text{A.3})$$

$$\tau_s = \mu_t \frac{\partial V}{\partial z}$$

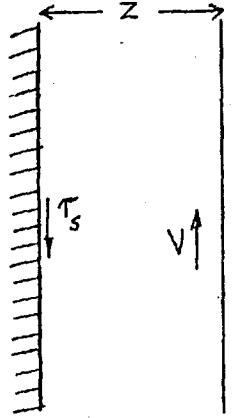
The Couette flow assumption [Launder and Spalding (1973)] enables the conservation equation of turbulent kinetic energy (eqn. 2.3.8) to be reduced to the following form:

$$G = C_D \rho \epsilon \quad (\text{A.5})$$

and the generation term, G may be assumed to be equal to the product of turbulent viscosity (μ_t) and the velocity gradient normal to the wall, thus:

$$\mu_t \left(\frac{\partial V}{\partial z} \right)^2 = C_D \rho \epsilon \quad (\text{A.6})$$

By replacing ϵ with $(C_\mu \rho k^2)/\mu_t$ (eqn. 2.3.11) and introducing



τ_s in place of $\frac{\partial V}{\partial z}$, eqn. (A.6) becomes:

$$\frac{\tau_s^2}{\mu_t} = \frac{C_D \rho C_\mu \rho k^2}{\mu_t}$$

$$k = \frac{\tau_s}{\rho} (C_\mu C_D)^{-\frac{1}{2}} \quad (A.7)$$

$$k^{\frac{1}{2}} = \frac{\tau_s}{\rho V_\tau} (C_\mu C_D)^{-\frac{1}{4}} \quad (A.8)$$

$$\tau_s = \rho k^{\frac{1}{2}} (C_\mu C_D)^{\frac{1}{4}} V_\tau \quad (A.9)$$

The substitution of V_τ , using the universal log-law relationship (eqn.A.1) yields the expressions for shear stress to be used in V-momentum equation:

$$\begin{aligned} \tau_s &= \rho k^{\frac{1}{2}} (C_\mu C_D)^{\frac{1}{4}} V / \ln(8.8z^+) \text{ for } z^+ > 11.63 \\ \tau_s &= \rho k^{\frac{1}{2}} (C_\mu C_D)^{\frac{1}{4}} V / z^+ \text{ for } z^+ \leq 11.63 \end{aligned} \quad (A.10)$$

By combining eqn. (A.7) with eqn. (A.3), the value of z^+ may be re-written in terms of k as follows:

$$z^+ = \frac{\rho k^{\frac{1}{2}} (C_\mu C_D)^{\frac{1}{4}}}{\mu} \quad (A.11)$$

Near-wall treatment of the dissipation term in k-conservation equation (2.3.8)

With the use of eqn.(2.3.11), the value of ϵ in the dissipation

term of eqn. (2.3.8) may be replaced by $(C_\mu \rho k^2 / \mu_t)$ to give the following expression:

$$\begin{aligned} \text{Dissipation term} &= C_D \rho \epsilon = C_D \rho \frac{C_\mu \rho k^2}{\mu_t} \\ &= \frac{\rho^2 C_\mu C_D k^2 V}{\tau_s z} \end{aligned}$$

By substituting τ_s in the above equation with the values given by eqn. (A.9), the expression emerged will be used in turbulent kinetic energy conservation equation:

$$\text{Dissipation term} = \rho (C_\mu C_D)^{\frac{3}{4}} k^{\frac{3}{2}} \ln (8.8z^+) / (.437z) \text{ for } z^+ > 11.63$$

$$\text{Dissipation term} = \rho (C_\mu C_D)^{\frac{3}{4}} k^{\frac{3}{2}} z^+ / z \text{ for } z^+ \leq 11.63$$

(A.12)

Near-wall dissipation rate of turbulent kinetic energy

To calculate ϵ near the wall, the first step is to write down an expression for μ_t in terms of k and the dissipation length scale (ℓ) where ℓ is defined as

$$\ell = \frac{k^{\frac{3}{2}}}{\epsilon} \quad (\text{A.13})$$

and

$$\mu_t = C_\mu \rho k^{\frac{1}{2}} \ell \quad (\text{A.14})$$

The substitution of eqn. (A.13) into eqn. (A.14) yields:

$$\epsilon = \frac{\mu_t^3}{C_\mu^3 \rho \ell^4} \quad (\text{A.15})$$

This expression is employed to eliminate ϵ from eqn. (A.6),
thus:

$$\begin{aligned}\mu_t \left(\frac{\partial V}{\partial z} \right)^2 &= C_D \rho \frac{\mu_t^3}{C_\mu^3 \rho^3 \ell^4} \\ \mu_t &= C_\mu^{\frac{3}{2}} C_D^{-\frac{1}{2}} \rho \ell^2 \frac{\partial V}{\partial z}\end{aligned}\tag{A.16}$$

From the mixing length (L) hypothesis, the turbulent viscosity is given by the following expression:

$$\mu_t = \rho L^2 \frac{\partial V}{\partial z}\tag{A.17}$$

In Couette flow analysis, L may be assumed to be directly proportional to the distance from the wall, i.e.

$$L = .437z\tag{A.18}$$

The substitution of eqn. (A.18) into eqn. (A.17) yields:

$$\mu_t = \rho (.437)^2 z^2 \frac{\partial V}{\partial z}\tag{A.19}$$

By equating the expression given by (A.19) with that by (A.16) the following result emerges:

$$\ell = .437z C_\mu^{-\frac{3}{4}} C_D^{\frac{1}{4}}\tag{A.20}$$

The combination of eqn. (A.13) with eqn. (A.20) will give an expression for the dissipation rate (ϵ) in the near-wall region, i.e.

$$\boxed{\epsilon = \frac{k^{\frac{3}{2}} C_\mu^{\frac{3}{4}}}{.437z C_D^{\frac{1}{4}}}}\tag{A.21}$$

The relationship between the dissipation Schmidt number and other turbulent constants

In order to find this relationship, the Couette-flow assumption is first used to reduce the conservation equation of ϵ (eqn. 2.3.9) to the following form:

$$\frac{\partial}{\partial z} \left[\frac{\mu_{\text{eff}}}{\delta_{\epsilon}} \frac{\partial \epsilon}{\partial z} \right] = \frac{C_1 \epsilon G}{k} - \frac{C_2 \rho \epsilon^2}{k} \quad (\text{A.22})$$

The substitution of G from eqn. A.5 yields:

$$\frac{\partial}{\partial z} \left[\frac{\mu_{\text{eff}}}{\delta_{\epsilon}} \frac{\partial \epsilon}{\partial z} \right] = (C_2 - C_1 C_D) \frac{\rho \epsilon^2}{k} \quad (\text{A.23})$$

The assumption of a uniform stress-layer near the wall will allow the term on the left-hand side to be written as $\frac{\mu_{\text{eff}}}{\delta_{\epsilon}} \frac{\epsilon}{z^2}$. If μ_t is taken to be very much larger than μ , eqn. (A.23) will become:

$$\frac{\mu_t}{\delta_{\epsilon}} \frac{\epsilon}{z^2} = (C_2 - C_1 C_D) \frac{\rho \epsilon^2}{k}$$

$$\delta_{\epsilon} = \frac{\mu_t k}{(C_2 - C_1 C_D) z^2 \rho \epsilon} \quad (\text{A.24})$$

By using eqn. (A.21) and replacing μ_t by $(C_{\mu} \rho k^2)/\epsilon$ the following equation results:

$$\delta_{\epsilon} = \frac{(.437)^2 C_D^{\frac{1}{2}}}{(C_2 - C_1 C_D) C_{\mu}^{\frac{1}{2}}} \quad (\text{A.25})$$

Appendix B: Derivation of the finite-difference equations

The finite-difference equations are derived by performing an integration on the governing differential equations over the control volume displayed in fig. 3.2.2. The staggered grid arrangement employed in the present procedure has resulted in the control volume being different for each of the dependent variables V, W and ϕ as shown in fig. B.1 (p. 207). In each control volume, the subscripts N, S, E and W (shown here only for the ϕ -cell) refer respectively to the points north, south, east and west of the point P where the solution is sought. The smaller letters n, s, e and w denote the four control volume boundaries which lie exactly midway between P and N, S, E and W respectively.

In the derivation, the variation of ϕ is assumed to be stepwise in time-direction and the backward difference is used to evaluate the time-derivatives. The calculations of the cross-stream convections employ the combination of the central-difference and upwind-difference formulae for the first order derivatives with the convected ϕ being taken as the arithmetic mean of the two ϕ 's along its side. For diffusion calculation, the linear variation of ϕ between grid points is assumed, except when the high-lateral-flux modification dictates otherwise.

The governing differential equations have been given in section 2.6, and they are:

Equation for conservation of ϕ 's (eqn. 2.6.2)

$$\begin{aligned} \frac{\partial(\rho\phi)}{\partial t} + \frac{\partial}{\partial z}(\rho W\phi) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V\phi) \\ = \frac{\partial}{\partial z} \left(\frac{\mu_{\text{eff}}}{\delta_{\phi}} \frac{\partial \phi}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\mu_{\text{eff}}}{\delta_{\phi}} \frac{\partial \phi}{\partial r} \right) + P_{\phi} + S_{\phi} \end{aligned}$$

The continuity equation (2.6.1)

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial z}(\rho W) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r V) = 0$$

The equations are integrated term by term and the results when assembled will yield the finite-difference equations.

B.1 Equation for conservation of ϕ 's

Integration of the first term

$$\frac{1}{\Delta t} \int_C \frac{\partial}{\partial t}(\rho \phi) dz r dr dt = \left(\frac{\Delta z \Delta r}{\Delta t} \rho \phi \right)_P - \left(\frac{\Delta z \Delta r}{\Delta t} \rho \phi \right)_U \quad (B.1)$$

where $\frac{1}{\Delta t} \int_C$ indicates the integration over the control volume divided by the Δt increment of time.

The present-step term in eqn. B.1 $\left[\left(\frac{\Delta z \Delta r}{\Delta t} \rho \phi \right)_P \right]$ is evaluated with the use of continuity equation. By integrating the continuity equation term by term, the following result may be obtained:

$$\frac{1}{\Delta t} \int_C \frac{\partial \rho}{\partial t} dz r dr dt = \left(\frac{\Delta z \Delta r}{\Delta t} \rho \right)_P - \left(\frac{\Delta z \Delta r}{\Delta t} \rho \right)_U$$

$$\frac{1}{\Delta t} \int_C \frac{\partial(\rho W)}{\partial z} dz r dr dt = \Delta r(\rho W)_e - \Delta r(\rho W)_w$$

$$\frac{1}{\Delta t} \int_C \frac{1}{r} \frac{\partial}{\partial r}(\rho r V) dz r dr dt = \Delta z(\rho V)_n - \Delta z(\rho V)_s$$

Thus

$$\begin{aligned} \left(\frac{\Delta z \Delta r}{\Delta t} \rho \right)_P &= \left(\frac{\Delta z \Delta r}{\Delta t} \rho \right)_U - \Delta r(\rho W)_e + \Delta r(\rho W)_w \\ &\quad - \Delta z(\rho V)_n + \Delta z(\rho V)_s \end{aligned} \quad (B.2)$$

Substitute (B.2) in (B.1) to yield:

$$\begin{aligned}
 \frac{1}{\Delta t} \int_C \frac{\partial}{\partial t}(\rho \phi) dz r dr dt &= \left[(\rho r \frac{\Delta z \Delta r}{\Delta t})_U - 2 \frac{\Delta r}{2} (\rho W r)_e + 2 \frac{\Delta r}{2} (\rho W r)_w \right. \\
 &\quad \left. - 2 \frac{\Delta z}{2} (\rho r V)_n + 2 \frac{\Delta z}{2} (\rho r V)_s \right] \phi_P - (\rho r \frac{\Delta z \Delta r}{\Delta t})_U \phi_U \\
 &= (F_U - 2 L_e^Z + 2 L_w^Z - 2 L_n^r + 2 L_s^r) \phi_P - F_U \phi_U \quad (B.3)
 \end{aligned}$$

Integration of other terms

$$\begin{aligned}
 \frac{1}{\Delta t} \int_C \frac{\partial}{\partial z}(\rho W \phi) dz r dr dt &= (\rho W r \Delta r \phi)_e - (\rho W r \Delta r \phi)_w \\
 &= \frac{\Delta r}{2} (\rho W r)_e (\phi_E + \phi_P) - \frac{\Delta r}{2} (\rho W r)_w (\phi_P + \phi_W) \\
 &= L_e^Z (\phi_E + \phi_P) - L_w^Z (\phi_P + \phi_W) \quad (B.4)
 \end{aligned}$$

$$\begin{aligned}
 \frac{1}{\Delta t} \int_C \frac{1}{r} \frac{\partial}{\partial r}(\rho r V \phi) dz r dr dt &= (\rho V r \Delta z \phi)_n - (\rho V r \Delta z \phi)_s \\
 &= \frac{\Delta z}{2} (\rho r V)_n (\phi_N + \phi_P) - \frac{\Delta z}{2} (\rho r V)_s (\phi_P + \phi_S) \\
 &= L_n^r (\phi_N + \phi_P) - L_s^r (\phi_P + \phi_S) \quad (B.5)
 \end{aligned}$$

$$\begin{aligned}
 \frac{1}{\Delta t} \int_C \frac{\partial}{\partial z} \left(\frac{\mu_{\text{eff}}}{\delta \phi} \frac{\partial \phi}{\partial z} \right) dz r dr dt &= (r \Delta r \frac{\mu_{\text{eff}}}{\delta \phi} \frac{\partial \phi}{\partial z})_e - (r \Delta r \frac{\mu_{\text{eff}}}{\delta \phi} \frac{\partial \phi}{\partial z})_w \\
 &= \left(\frac{r \Delta r \mu_{\text{eff}}}{\Delta z \delta \phi} \right)_e (\phi_E - \phi_P) - \left(\frac{r \Delta r \mu_{\text{eff}}}{\Delta z \delta \phi} \right)_w (\phi_P - \phi_W) \\
 &= T_e^z (\phi_E - \phi_P) - T_w^z (\phi_P - \phi_W) \quad (\text{B.6})
 \end{aligned}$$

$$\begin{aligned}
 \frac{1}{\Delta t} \int_C \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\mu_{\text{eff}}}{\delta \phi} \frac{\partial \phi}{\partial r} \right) dz r dr dt &= (\Delta z r \frac{\mu_{\text{eff}}}{\delta \phi} \frac{\partial \phi}{\partial r})_n - (\Delta z r \frac{\mu_{\text{eff}}}{\delta \phi} \frac{\partial \phi}{\partial r})_s \\
 &= \left(\frac{r \Delta z \mu_{\text{eff}}}{\Delta r \delta \phi} \right)_n (\phi_N - \phi_P) - \left(\frac{r \Delta z \mu_{\text{eff}}}{\Delta r \delta \phi} \right)_s (\phi_P - \phi_S) \\
 &= T_n^r (\phi_N - \phi_P) - T_s^r (\phi_P - \phi_S) \quad (\text{B.7})
 \end{aligned}$$

$$\frac{1}{\Delta t} \int_C P_\phi dz r dr dt = P_\xi \quad (\text{B.8})$$

$$\begin{aligned}
 \frac{1}{\Delta t} \int_C S_\phi dz r dr dt &= (S_\phi r \Delta r \Delta z)_P \\
 &= S_U + S_P \phi_P \quad (\text{B.9})
 \end{aligned}$$

Assemble equations (B.3) to (B.9) to give:

$$(F_U - 2 L_e^z + 2 L_w^z - 2 L_n^r + 2 L_s^r) \phi_P - F_U \phi_U + L_e^z (\phi_E + \phi_P) - L_w^z (\phi_P + \phi_W)$$

$$+ L_n^r (\phi_N + \phi_P) - L_s^r (\phi_P + \phi_S) = T_e^z (\phi_E - \phi_P) - T_w^z (\phi_P - \phi_W) + T_n^r (\phi_N - \phi_P) \\ - T_s^r (\phi_P - \phi_S) + P_\xi + S_U + S_P \phi_P$$

Rearrange the above equation into the following form:

$$(F_U - L_e^z + L_w^z - L_n^r + L_s^r + T_e^z + T_w^z + T_n^r + T_s^r - S_P) \phi_P \\ = (T_n^r - L_n^r) \phi_N + (T_s^r + L_s^r) \phi_S + (T_e^z - L_e^z) \phi_E + (T_w^z + L_w^z) \phi_W + F_U \phi_U + S_U + P_\xi \\ [(T_n^r - L_n^r) + (T_s^r + L_s^r) + (T_e^z - L_e^z) + (T_w^z + L_w^z) + F_U - S_P] \phi_P \\ = (T_n^r - L_n^r) \phi_N + (T_s^r + L_s^r) \phi_S + (T_e^z - L_e^z) \phi_E + (T_w^z + L_w^z) \phi_W + (F_U \phi_U + S_U) + P_\xi \\ (A_N + A_S + A_E + A_W + F_U - S_P) \phi_P = A_N \phi_N + A_S \phi_S + A_E \phi_E + A_W \phi_W + B + U \quad (B.10) \\ \phi_P = A_N \phi_N + A_S \phi_S + A_E \phi_E + A_W \phi_W + B \phi + U \phi \quad (B.11)$$

In the above equation the coefficient T's is replaced $\bar{T}$ where the latter is calculated from the upwind difference assumption as follows:

$$T's = \frac{1}{2} [T + |L| + |T - |L||] \quad (B.12)$$

The coefficient U^ϕ in equation (B.11) is zero for most ϕ equations except the two momentum equations in which it represents the term expressing the effect of pressure gradients; i.e.:

$$U^\phi = D^\phi \Delta P \quad (B.13)$$

Thus equation (B.11) may be rewritten for all governing equations in the following form:

Momentum equations:

$$W_P = A_{NN}^W + A_{SS}^W + A_{EE}^W + A_{WW}^W + B^W + D^W (P_P - P_W) \quad (B.14)$$

$$V_P = A_{NN}^V + A_{SS}^V + A_{EE}^V + A_{WW}^V + B^V + D^V (P_P - P_S)$$

Equation for other dependent variables (ϕ 's):

$$\phi_P = A_{NN}^\phi + A_{SS}^\phi + A_{EE}^\phi + A_{WW}^\phi + B^\phi \quad (B.15)$$

B.2 The continuity equation

In the derivation of the finite difference equation to replace the continuity equation, the following relationships⁽¹⁾ are used to relate the dependent variable (P') to the estimated (V^*, W^*) the actual (V, W) velocity fields and the velocity corrections (V', W'):

$$\begin{aligned} V'_n &= V_n - V_n^* = D_n^V (P'_N - P'_P) \\ V'_s &= V_s - V_s^* = D_s^V (P'_P - P'_S) \\ W'_e &= W_e - W_e^* = D_e^W (P'_E - P'_P) \\ W'_w &= W_w - W_w^* = D_w^W (P'_P - P'_W) \end{aligned} \quad (B.16)$$

(1) The derivation appears in Appendix B.3

In subsonic compressible flow, the density may be calculated from the assumed perfect gas law.

$$\rho^* = KP^* \quad (B.17)$$

$$\text{where } K = \frac{1}{RT \sum_j \frac{m_j}{M_j}} \quad (B.18)$$

Here ρ^* and P^* denote the estimated density and pressure which are related to their actual values (ρ and P) via the corrections ρ' and P' as follows:

$$\rho = \rho^* + \rho' \quad (B.19)$$

$$P = P^* + P' \quad (B.20)$$

With the use of the information given by equations (B.16) to (B.20), the continuity equation may be integrated term by term to give the finite-difference equation with P' as the dependent variable.

$$\begin{aligned} \frac{1}{\Delta t} \int_C \frac{\partial}{\partial t} dz r dr dt &= \left(\frac{\Delta z \Delta r}{\Delta t} \rho r \right)_P - \left(\frac{\Delta z \Delta r}{\Delta t} \rho r \right)_U \\ &= \left[\frac{\Delta z \Delta r}{\Delta t} r (\rho^* + \rho') \right]_P - \left(\frac{\Delta z \Delta r}{\Delta t} \rho r \right)_U \\ &= \left[\frac{\Delta z \Delta r}{\Delta t} r (KP^* + KP') \right]_P - \left(\frac{\Delta z \Delta r}{\Delta t} \rho r \right)_U \\ &= \left[\frac{\Delta z \Delta r}{\Delta t} r KP' \right]_P + \left(\frac{\Delta z \Delta r}{\Delta t} r KP^* \right)_P - \left(\frac{\Delta z \Delta r}{\Delta t} \rho r \right)_U \end{aligned}$$

$$= S_P P'_P + F_D - F_U \quad (B.21)$$

$$\begin{aligned} \frac{1}{\Delta t} \int_C \frac{\partial(\rho W)}{\partial z} dz r dr dt &= \frac{1}{\Delta t} \int_C \frac{\partial}{\partial z} [(\rho^* + \rho')(W^* + W')] dz r dr dt \\ &= \frac{1}{\Delta t} \int_C \frac{\partial}{\partial z} (\rho^* W^* + \rho^* W' + \rho' W^*) dz r dr dt \\ &= \frac{1}{\Delta t} \int_C \frac{\partial}{\partial z} (K_P^* W^* + K_P^* W' + K_P' W^*) dz r dr dt \\ &= [r \Delta r (K_P^* W^* + K_P^* W' + K_P' W^*)]_e - [r \Delta r (K_P^* W^* + K_P^* W' + K_P' W^*)] \\ &= [(\rho^* W^* r \Delta r)_e + (\rho^* r \Delta r)_e D_e^W (P'_E - P'_P) + (K_P r \Delta r W^*)_e \left(\frac{P'_P + P'_E}{2} \right)] \\ &\quad - [(\rho^* W^* r \Delta r)_w + (\rho^* r \Delta r)_w D_w^W (P'_P - P'_W) + (K_P r \Delta r W^*)_w \left(\frac{P'_P + P'_W}{2} \right)] \\ &= 2L_e^Z + G_e^Z (P'_E - P'_P) + Q_e^Z (P'_P + P'_E) \\ &\quad - 2L_w^Z - G_w^Z (P'_P - P'_W) - Q_w^Z (P'_P + P'_W) \quad (B.22) \end{aligned}$$

$$\begin{aligned} \frac{1}{\Delta t} \int_C \frac{\partial(\rho r V)}{\partial r} dr r dr dt &= [(\rho^* V^* r \Delta z)_n + (\rho^* r \Delta z)_n D_n^V (P'_N - P'_P) + (K_P r \Delta z V^*)_n \left(\frac{P'_P + P'_N}{2} \right)] \\ &\quad - [(\rho^* V^* r \Delta z)_s + (\rho^* r \Delta z)_s D_s^V (P'_P - P'_S) + (K_P r \Delta z V^*)_s \left(\frac{P'_P + P'_S}{2} \right)] \\ &= 2L_n^r + G_n^r (P'_N - P'_P) + Q_n^r (P'_P + P'_N) \end{aligned}$$

$$- 2L_s^r - G_s^r(P_P' - P_S') - Q_s^r(P_P' + P_S') \quad (B.23)$$

Equations (B.21), (B.22) and (B.23) are recombined to yield:

$$\begin{aligned} & (S_P P_P' + F_D - F_U) + [2L_e^Z + G_e^Z(P_E' - P_P') + Q_e^Z(P_P' + P_E') - 2L_w^Z - G_w^Z(P_P' - P_W') - Q_w^Z(P_P' + P_W')] \\ & + [2L_n^r + G_n^r(P_N' - P_P') + Q_n^r(P_P' + P_N') - 2L_s^r - G_s^r(P_P' - P_S') - Q_s^r(P_P' + P_S')] \\ & = 0 \end{aligned}$$

$$[(-G_e^Z + Q_e^Z) + (-G_w^Z - Q_w^Z) + (-G_n^r + Q_n^r) + (-G_s^r - Q_s^r) - S_P]P_P'$$

$$= (-G_e^Z - Q_e^Z)P_E' + (-G_w^Z + Q_w^Z)P_W' + (-G_n^r - Q_n^r)P_N' + (-G_s^r + Q_s^r)P_S'$$

$$- 2L_e^Z + 2L_w^Z - 2L_n^r + 2L_s^r - F_D + F_U \quad (B.24)$$

$$A_{P_P'} = A_{E_E'} + A_{W_W'} + A_{N_N'} + A_{S_S'} + B$$

$$P_P' = A_{E_E'}^P + A_{W_W'}^P + A_{N_N'}^P + A_{S_S'}^P + B^P \quad (B.25)$$

It may be observed that as the terms Q's represent the convective contribution, the upwind difference technique is used in their calculation, i.e.:

$$Q's = \frac{1}{2} (|Q| + Q) \quad (B.26)$$

B.3 An improved version of velocity-pressure correction (B.16) relationships

A more accurate form of equations (B.16) is used in the present computation. In the derivation equation (B.10) is written for W-velocity component as follows:

$$(A_N + A_S + A_E + A_W + F_U - S_P)W_P = A_N W_N + A_S W_S + A_E W_E + A_W W_W + B + D'^W (P_P - P_W)$$

or

$$[(\sum_j A_j) + F_U - S_P]W_P = (\sum_j A_j W_j) + B + D'^W (P_P - P_W) \quad (B.27)$$

As both the actual and estimated (V^*, W^*) velocity fields satisfy the momentum equation, equation similar to that given by (B.27) may be written for W^* :

$$[(\sum_j A_j) + F_U - S_P]W_P^* = (\sum_j A_j W_j^*) + B + D'^W (P_P^* - P_W^*) \quad (B.28)$$

The subtraction of (B.28) from (B.27) will leave the following equation:

$$[(\sum_j A_j) + F_U - S_P][W_P - W_P^*] = \sum_j A_j (W_j - W_j^*) + D'^W [(P_P - P_P^*) - (P_W - P_W^*)]$$

Introducing P' as the difference between the actual and estimated pressure, the equation may be rearranged to give:

$$\left[\left(\sum_j A_j \right) + F_U - S_P \right] W_P = \left[\left(\sum_j A_j \right) + F_U - S_P \right] W_P^* + D^W (P_P' - P_W') + \sum_j [A_j (W_j - W_j^*)] \quad (\text{B.29})$$

If the last term on the right hand side of the above equation is neglected, the resulting equation will give a relationship between the pressure and velocity corrections (eqn. B.16) i.e.:

$$W_P' = W_P - W_P^* = D^W (P_P' - P_W') \quad (\text{B.30})$$

When a very small time-step is employed, the equation prescribes the relationship quite accurately. To get the same accuracy with the use of a bigger step, the previously neglected term which contains the unknown W_j must be implicitly included by assuming that $(W_j - W_j^*)$ is equal to $(W_P - W_P^*)$. Hence,

$$(F_U - S_P) W_P = (F_U - S_P) W_P^* + D^W (P_P' - P_W')$$

or

$$W_P = W_P^* + \frac{D^W}{(F_U - S_P)} (P_P' - P_W') \quad (\text{B.31})$$

Similarly the following equation may be written for V_P :

$$V_P = V_P^* + \frac{D^V}{(F_U - S_P)} (P_P' - P_S') \quad (\text{B.32})$$

Equations (B.31) and (B.32), not (B.30) are used in the present investigation in place of eqn. (B.16).

APPENDIX C Analyses used to obtain the velocity and temperature
at the nozzle exit

C.1 The calculation of the velocity of discharge

The problem considered involves the isothermal, unsteady discharge of nitrogen from an enclosure into stagnant atmosphere through a small nozzle. The analysis employs the perfect gas law to relate the mass of the content in the enclosure to the fluid properties and states, viz:

$$P_c V_c = \frac{m_c R T_{atm}}{M_{N_2}} \quad (C.1.1)$$

where P_c, V_c, m_c represent the enclosure pressure, enclosure volume and the mass of N_2 inside the enclosure respectively; M_{N_2} is nitrogen molecular weight, T_{atm} the atmospheric temperature and R , the universal gas constant.

Eqn. (C.1.1) is differentiated with respect to time and the resulting expression is rearranged to yield:

$$\frac{dm_c}{dt} = \left(\frac{M_{N_2} V_c}{R T_{atm}} \right) \frac{dP_c}{dt} \quad (C.1.2)$$

If the velocity is assumed to be uniform across the nozzle exit the rate of discharge, $\frac{dm_c}{dt}$ may be related to the nozzle velocity of discharge ($w_{o,I}$), nozzle diameter (d) and fluid density through the continuity equation, i.e.:

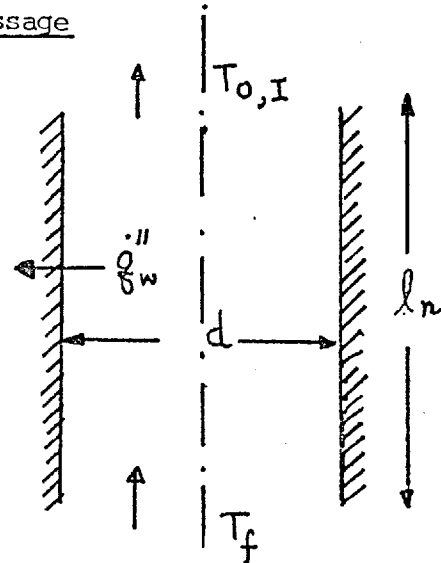
$$\frac{dm_c}{dt} = \frac{\rho \pi d^2 w_{o,I}}{4} \quad (C.1.3)$$

The substitution of eqn. (C.1.3) in eqn. (C.1.2) will give the following expression which can be used to obtain $W_{O,I}$ from the measurement of P_c .vs. t :

$$W_{O,I} = \left(\frac{M_N V_c}{RT_{atm}} \right) \left(\frac{4}{\rho \pi 4 d^2} \right) \frac{dP_c}{dt} \quad (C.1.4)$$

C.2 Heat transfer for flow through the nozzle passage

The present problem studies the flow of hot gases through a small nozzle passage. In the calculation of the temperature drop along the passage, the following assumptions have been made:



- (i) the flow is one-dimensional
- (ii) the hot gases at the nozzle inlet are at the flame temperature, T_f (1)
- (iii) both the velocity and temperature across the nozzle outlet are uniform and equal to $W_{O,I}$ and $T_{O,I}$ respectively.

Thus the following heat-balance equation may be written:

$$\dot{q}_w'' \pi d l_N = \frac{\rho \pi d^2 W_{O,I}}{4} C_P (T_f - T_{O,I}) \quad (C.2.1)$$

(1) T_f is obtained from the experimental data of Kaimatov and Bauer (1966)

where C_p and ρ are the specific heat and density of the fluid

d and ℓ_N are the diameter and length of the nozzle passage

$\dot{q}''_w$, the heat transfer rate through the wall, may be evaluated using the following expression:

$$\overline{Nu} = \frac{\dot{q}''_w d}{k_g T_b} \quad (C.2.2)$$

where k_g is the thermal conductivity of hot gases, $\overline{Nu}$ the average Nusselt number and T_b the bulk temperature.

By substituting eqn. (C.2.2) in eqn. (C.2.1), the following equation results:

$$\overline{Nu} = \frac{T_f - T_{O,I}}{T_b} \frac{d}{4\ell_N} \overline{Re} \overline{Pr} \quad (C.2.3)$$

Here $\overline{Re}$ and $\overline{Pr}$ which are the average Reynolds and Prandtl numbers are defined as:

$$\overline{Re} = \frac{\rho^w_{O,I} d}{\mu} \quad (C.2.4)$$

$$\overline{Pr} = \frac{C_p \mu}{k_g} \quad (C.2.5)$$

where μ is the laminar viscosity of fluid.

Eqn. (C.2.3) is used in the present investigation to obtain the $\overline{Nu}$ vs. $\overline{Re}$ relationship.

APPENDIX D: Tables of experimental results

Table D.1 The discharge coefficient of the nozzle from
the 'cold' flow tests

Time (ms)	P_c (kN/m ²)	$\frac{dP_c}{dt}$ (kN/m ² s)	$(W_{O,I})^I$ (m/s)	$W_{O,I}$ (m/s)	Re	C_d
0	131.50					
50	121.85	182.84	180.0	124.1	250	.69
100	114.91	132.05	147.8	89.6	180	.61
150	108.81	89.73	110.5	60.9	123	.55
200	105.43	56.72	81.8	38.5	77	.47
0	123.53					
50	116.42	155.76	155.6	105.7	213	.68
100	109.65	101.58	116.5	69.0	139	.59
150	105.76	71.11	85.2	48.3	97	.57
200	103.05	41.48	52.6	28.2	57	.53
0	126.07					
50	116.76	155.77	157.2	105.7	213	.67
100	110.00	120.20	118.8	81.6	164	.65
150	105.93	81.26	86.8	55.2	111	.63
200	103.39	52.48	57.7	35.6	72	.62

Table D.2: Temperature and velocity results (with the explosion cylinder consisting of 9% CH₄, 22% O₂ and 69% N₂ by volume

Time (ms)	P _c kN/m ²	W _{O,I} (m/s)	T _T (°K)			T _{O,I} (°K)
			(with 75µm)	(with 100µm)	(with 125µm)	
5.5	101.36	0.0	295	295	295	295
6	102.71	28.9	393	318	318	433
7	103.56	36.7	558	411	389	628
8	104.40	43.1	698	496	466	782
9	105.42	49.6	819	575	530	928
10	107.11	58.8	938	654	587	1072
11	109.31	68.8	1023	735	655	1213
12	114.05	86.1	1123	812	731	1355
13	118.63	99.6	1215	895	798	1474
14	127.42	120.6	1302	981	863	1576
15	136.06	132.0	1394	1065	927	1687
16	144.87	151.8	1485	1151	1000	1810
17	151.98	162.1	1561	1232	1065	1890
18	153.67	164.4	1633	1310	1125	1969
19	153.67	164.4	1693	1380	1186	2013
20	151.98	162.1	1765	1451	1255	2070
21	146.22	153.8	1821	1514	1306	2130
22	136.01	132.0	1839	1562	1354	2136
23	118.63	99.6	1865	1598	1396	2095
24	110.16	72.0	1865	1617	1417	2084

$$W_{O,I} = -.29811E+2+.25547E+5t-.45795E+7t^2+.39459E+9t^3-.10291E+11t^4$$

$$T_{O,I} = -.14255E+3+.74512E+5t+.75820E+7t^2-.28940E+9t^3$$

where t is the time measured in milliseconds from the instant the prepared mixture inside the explosion cylinder is spark-ignited.

Table D 3: $\overline{Nu}$ vs. $\overline{Re}$ obtained from one-dimensional analysis of the flow through the nozzle passage using the results tabulated in Table D.2

Time (ms)	No. (m/s)	$T_{O,T}$ ($^{\circ}K$)	$\overline{Re}$	$\overline{Nu}$
6	28.9	433	446	16.9
7	36.7	628	501	15.4
8	43.1	782	532	13.8
9	49.6	928	566	12.4
10	58.8	1072	623	11.4
11	68.8	1213	677	10.3
12	86.1	1355	795	9.77
13	99.6	1474	874	8.82
14	120.69	1576	1005	8.37

Table D.4: Temperature and velocity results for other cases

D.4.1 with the explosion cylinder consisting of 9.8% CH₄
and air by volume

Time (ms)	P _c (kN/m ²)	W _{O,I} (m/s)	Re	Nu	T _{O,I} (°K)
1.5	101.36	0	-	-	295
1.9	103.84	39	481	15.8	593
3.1	105.15	48	533	13.9	786
4.2	106.01	53	554	13.1	898
5.5	106.87	58	580	12.3	989
6.6	109.63	70	640	11.1	1188
7.8	111.35	77	677	10.5	1271
8.9	113.77	85	716	10.0	1360

$$W_{O,I} = -.16374E+3+.18039E+6T-.53820E+8t^2+.67979E+10t^3-.30080E+12t^4$$

$$T_{O,I} = -.27865E+4+.37960E+7t-.15496E+10t^2+.30270E+12t^3-.2782E+14t^4$$

$$+.97116E+15t^5$$

D.4.2 with the explosion cylinder consisting of 9% CH₄
and air by volume

Time (ms)	P _c (kN/m ²)	W _{O,I} (m/s)	Re	Nu	T _{O,I} (°K)
3.2	101.36	0	-	-	295
5.5	102.25	24	-	-	389
6.5	102.53	27	-	-	374
7.5	102.87	31	439	17.1	421
8.5	103.24	34	459	16.7	489
9.5	103.77	38	479	15.9	606
10.5	104.67	45	515	14.5	772

$$W_{O,I} = -.52543E+3+.27609E+6t-.15373E+8t^2+.42025E+10t^3-.12586E+12t^4$$

$$T_{O,I} = -.11415E+3+.17788E+6t-.24033E+8t^2+.97337E+9t^3+.44575E+11t^4$$

D.4.3 with the explosion cylinder consisting of 8% CH₄
and air by volume

Time (ms)	P _c (kN/m ²)	W _{O,I} (m/s)	$\overline{Re}$	$\overline{Nu}$	T _{O,I} (°K)
5.0	101.36	0	-	-	295
5.2	101.84	18.0	-	-	316
6.2	102.05	21.0	-	-	333
7.2	102.18	23.0	-	-	348
8.2	102.34	25.0	-	-	375
9.2	102.53	27.0	426	17.4	398
10.2	102.80	30.0	457	16.8	481
11.2	103.29	34.4	481	15.8	571
12.2	103.84	39.0	509	14.7	675
13.2	104.67	45.1	542	13.5	821

$$W_{O,I} = -.48560E+3+.22434E+6t-.35356E+8t^2+.25593E+10t^3-.65315E+11t^4$$

$$T_{O,I} = -.98206E+3+.61844E+6t-.10689E+9t^2+.78628E+10t^3-.19181E+12t^4$$