

COMBUSTION IN LAMINAR MIXING REGIONS  
AND BOUNDARY LAYERS

Thesis by  
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To  
My Wife, Alberta  
and to  
Mary and Kevin

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## ABSTRACT

The governing relations for gaseous flow systems with chemical reaction are briefly discussed. A mixture of mechanically similar Maxwellian molecules is assumed and the general relations are then reduced to the simplified forms appropriate for reacting, laminar boundary layer type flow systems. One-step unopposed, "global" reactions following first-order, second-order, and third-order kinetics are considered.

The simplified governing relations are transformed to an equivalent constant density plane by application of the Howarth transformation. A similarity function relating the specie concentrations to the local temperature is found for the case of equal Prandtl and Schmidt numbers. The similarity function is shown to be equal to the dimensionless streamwise velocity when the Prandtl and Schmidt numbers are both equal to unity. The remaining governing relations are then transformed to the Blasius plane in which the velocity field has known solutions. The energy equation is solved by an iteration process; a general analytic solution for the N'th approximation is obtained.

The analytic techniques developed are applied to the problems of combustion within laminar mixing regions and boundary layers. Temperature and concentration profiles are calculated and the dependence of the characteristic stay time upon the parameters of the system is determined. The application of the similarity techniques to the problem of chemical reaction within a hypersonic boundary layer is briefly discussed in an Appendix.

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## LIST OF SYMBOLS\*

A. English Characters

<u>Symbol</u>	<u>Page on which Introduced</u>	<u>Dimensions</u>	<u>Definition</u>
b	23	Cf. footnote, page 23.	So-called frequency factor: cf. page 23.
$c_{v_i}$	9	$\text{cm}^2/\text{sec}^2/^\circ\text{K}$	Specific heat at constant volume of the i'th chemical specie, per gram mass.
$c_v$	9	$\text{cm}^2/\text{sec}^2/^\circ\text{K}$	Equivalent specific heat at constant volume of the gas mixture, per gram mass of mixture.
$c_p$	20	$\text{cm}^2/\text{sec}^2/^\circ\text{K}$	Equivalent specific heat at constant pressure for the gas mixture, per gram mass of mixture.
$\vec{C}_0$	7	cm/sec	Local mass average velocity of the gas mixture: $\vec{C}_0 = \frac{1}{S} \sum_{\lambda} \rho_{\lambda} \vec{C}_{\lambda}^*$
$C_{0\alpha}$	13	cm/sec	The $\alpha$ -component of the local mass average velocity of the gas mixture.
$\vec{C}_i^*$	x	cm/sec	Average physical (or actual) velocity of the molecules (or atoms) of the i'th specie.
$\vec{C}_i$	7	cm/sec	Diffusion velocity, referred to $\vec{C}_0$ , of the molecules (or atoms) of the i'th specie: $\vec{C}_i = \vec{C}_i^* - \vec{C}_0 = \vec{C}_i - \vec{C}_0$

\* Symbols which are peculiar to an Appendix are defined in the appropriate Appendix and are excluded from this list.

## LIST OF SYMBOLS (Continued)

<u>Symbol</u>	<u>Page on which Introduced</u>	<u>Dimensions</u>	<u>Definition</u>
$C_1$	48	Dimensionless	Physical parameter related to the energy release during chemical reaction.
$C_2$	48	Dimensionless	Physical parameter related to the boundary conditions on the temperature.
$C_3$	49	$\text{cm}^{-1}$	Physical parameter related to properties of the flow system.
$\vec{d}_j$	11	$\text{gms}/\text{cm}^2/\text{sec}$	A flux vector for the j'th chemical specie; cf. page 12.
$D_i^T$	11	$\text{cm}^2/\text{sec}$	Multicomponent thermal diffusion coefficient.
$D_{ij}$	11	$\text{cm}^2/\text{sec}$	Multicomponent ordinary diffusion coefficient.
$D_{ij}$	16	$\text{cm}^2/\text{sec}$	Binary diffusion coefficient.
$D$	19	$\text{cm}^2/\text{sec}$	Coefficient of self-diffusion; also applicable to mixtures of mechanically similar molecules; cf. page 18.
$E$	23	$\text{ergs}/\text{gm-mole}$	Activation energy for a chemical reaction.
$f(\eta)$	61	Dimensionless	Blasius type dependent variable.
$F(x, y)$	54	Dimensionless	A dimensionless variable, expressed in various coordinate systems, which is utilized in a similarity solution.
$F(x, \eta)$	60		
$F(\eta)$	71		
$G_i(x, y)$	48	Dimensionless	A dimensionless specie concentration variable.

## LIST OF SYMBOLS (Continued)

<u>Symbol</u>	<u>Page on which Introduced</u>	<u>Dimensions</u>	<u>Definition</u>
$\hat{h}_i$	16	$\text{cm}^2/\text{sec}^2$	Total enthalpy per unit mass of the i'th chemical specie.
$\Delta H_f^0$	27	ergs/gm	Standard heat of formation at 298.16°K per gram of the i'th chemical specie.
$\overline{\Delta H}$	29	°K	Physical parameter related to the energy release during chemical reaction; cf. page 29.
$\vec{j}_i$	9	$\text{gms}/\text{cm}^2/\text{sec}$	Mass flux vector for the i'th chemical specie.
$K_i$	7	$\text{cc}^{-1}\text{sec}^{-1}$	Net rate of production per unit volume of molecules of the i'th chemical specie due to chemical reaction.
k	9	ergs/°K	Boltzmann's constant = $1.3804 \times 10^{-16}$ ergs/°K.
$k_f$	23	Cf. footnote, page 23.	Specific reaction rate coefficient.
$\mathcal{L}^{(N)}(\eta, x)$	74	Dimensionless	The N'th approximation to a heat release integral.
$m_i$	22	Dimensionless	Symbol for the i'th chemical specie.
$m^*$	23	Dimensionless	Order of the kinetics rate law followed by the reaction.
$m_i$	7	gms	Mass of a molecule of the i'th chemical specie.
m	19	gms	Mass of any molecule in a mixture of mechanically similar molecules.

## LIST OF SYMBOLS (Continued)

<u>Symbol</u>	<u>Page on which Introduced</u>	<u>Dimensions</u>	<u>Definition</u>
M	10	Dimensionless	Equivalent molecular weight of the gas mixture.
$n_i$	7	$\text{cc}^{-1}$	Number density of the molecules of the i'th chemical specie.
n	10	$\text{cc}^{-1}$	Number density of the gas mixture.
N	10	Dimensionless	Number of distinct chemical species in the gas mixture.
$\bar{N}$	22	Dimensionless	Number of distinct chemical species which take active part in the chemical reaction.
$P_i$	9	$\text{dynes/cm}^2$	Partial pressure of the i'th chemical specie.
p	10	$\text{dynes/cm}^2$	Local hydrostatic pressure of the gas mixture.
$\underline{\underline{P}}$	8	$\text{dynes/cm}^2$	Pressure tensor.
$P_{\alpha\alpha}$	14	$\text{dynes/cm}^2$	Diagonal scalar component of the pressure tensor.
$P_{\alpha\beta}$	14	$\text{dynes/cm}^2$	Non-diagonal scalar component of the pressure tensor.
	20	Dimensionless	Prandtl number = $c_p \mu / \lambda$
$\beta(r)$	116	Dimensionless	Parameter related to the Prandtl number.
$\vec{q}$	9	$\text{ergs/cm}^2/\text{sec}$	Heat flux vector; cf. page 16.
$Q^{(N)}(\eta, x)$	7.	Dimensionless	The N'th approximation to a dimensionless quantity related to the heat release integral.

## LIST OF SYMBOLS (Continued)

<u>Symbol</u>	<u>Page on which Introduced</u>	<u>Dimensions</u>	<u>Definition</u>
$r$	18	cm	Radial distance between two interacting molecules.
$\mathcal{R}$	10	ergs/ $^{\circ}$ K/gm-mole	Universal gas constant = $8.314 \times 10^7$ ergs/ $^{\circ}$ K/gm-mole.
$\zeta$	83	Dimensionless	Dimensionless streamwise coordinate.
$R^{(N)}(\eta, x)$	74	Dimensionless	The N'th approximation to a heat release integral.
$\underline{\underline{S}}$	13	sec $^{-1}$	Rate of shear tensor.
$S_{\alpha\beta}$	13	sec $^{-1}$	Scalar component of the rate of shear tensor.
Sc	20	Dimensionless	Schmidt number = $\mu/\rho D$
$s$	59	cm	Independent distance variable.
$t$	7	sec	Time
$t^*$	81	sec	Characteristic stay time.
$T$	9	$^{\circ}$ K	Local absolute temperature of the gas mixture.
$T_f$	29	$^{\circ}$ K	Adiabatic flame temperature for a stoichiometric combustible mixture.
$\underline{\underline{U}}$	13	Dimensionless	Unit tensor.
$\hat{U}_i$	9	cm $^2$ /sec $^2$	Total internal energy per unit mass of the i'th specie.

## LIST OF SYMBOLS (Continued)

<u>Symbol</u>	<u>Page on which Introduced</u>	<u>Dimensions</u>	<u>Definition</u>
$U(x, y)$	48	Dimensionless	Dimensionless streamwise velocity variable expressed in two different coordinate systems.
$U(\eta)$	61		
$u_o$	15	cm/sec	Actual streamwise velocity in the physical plane.
$u$	43	cm/sec	Streamwise velocity in the Howarth plane.
$V$	48	Dimensionless	Dimensionless transverse velocity.
$v_o$	15	cm/sec	Actual transverse velocity in the physical plane.
$v$	43	cm/sec	Transverse velocity in the Howarth plane.
$W$	59	cm/sec	A velocity parameter.
$w_o$	15	cm/sec	Actual velocity in the physical plane in the positive direction of the $z_o$ axis.
$w_i$	33	sec <sup>-1</sup>	Mass rate of removal per unit volume and per unit density of the i'th chemical specie due to chemical reaction.
$w_n$	27	sec <sup>-1</sup>	As above, for any reactant specie.
$w_p$	27	sec <sup>-1</sup>	Mass rate of production per unit volume and per unit density of the product specie due to chemical reaction.
$\vec{X}_i$	8	dynes/molecule	Force vector acting on molecules of the i'th chemical specie due to an external field.



## LIST OF SYMBOLS (Continued)

<u>Symbol</u>	<u>Page on which Introduced</u>	<u>Dimensions</u>	<u>Definition</u>
$X(x)$	73	Dimensionless	Dimensionless streamwise distance.
$x_0$	15	cm	Streamwise coordinate in the physical plane.
$x$	42	cm	Streamwise coordinate in the Howarth plane.
$x^*$	80	cm	Characteristic "flame attachment length".
$y_0$	15	cm	Transverse coordinate in the physical plane.
$y$	42	cm	Transverse coordinate in the Howarth plane.
$z_0$	15	cm	Coordinate in the physical plane which is normal to both the $x_0$ and the $y_0$ axis.
$z$	48	Dimensionless	Dimensionless local temperature in a region in which chemical reaction is occurring.
$z^{(0)}$	72	Dimensionless	Dimensionless local temperature in absence of chemical reaction.
$Z^{(N)}(\eta, x)$	74	Dimensionless	Variable quantity; cf. page 74.
<b>B. <u>Greek Characters</u></b>			
$\alpha$	18	$\text{gm-cm}^6/\text{sec}^2$	Force constant of proportionality for Maxwellian molecules.

## LIST OF SYMBOLS (Continued)

<u>Symbol</u>	<u>Page on which Introduced</u>	<u>Dimensions</u>	<u>Definition</u>
$\lambda$	16	ergs/cm/sec <sup>o</sup> K	Local coefficient of thermal conductivity for the gas mixture; molecules may be monatomic or polyatomic.
$\lambda^{\circ}$	19	ergs/cm/sec/ <sup>o</sup> K	Same as above except valid only for a gas mixture of monatomic, mechanically similar, Maxwellian molecules.
$\Lambda$	50	Dimensionless	Ratio of the streamwise velocity at the hot boundary to that at the cold boundary; $\Lambda \equiv u_{\infty}/u_c$
$\mu$	13	gm/cm/sec	Local coefficient of dynamic shear viscosity for the gas mixture.
$\nu$	44	cm <sup>2</sup> /sec	Kinematic viscosity of the cold free stream at temperature T <sub>I</sub> : $\nu \equiv \mu_{\infty}/\rho_{\infty}$
$\nu_i', \nu_i''$	22	Dimensionless	Reactant and product stoichiometric coefficients respectively for the i'th chemical specie.
$\rho_i$	16	gms/cc	Mass density of the i'th chemical specie.
$\rho$	7	gms/cc	Mass density of the gas mixture.
$\beta_i$	48	Dimensionless	Dimensionless activation energy.
$\delta_{\alpha\beta}$	13	Dimensionless	Kronecker delta; cf. page 14.

## LIST OF SYMBOLS (Continued)

<u>Symbol</u>	<u>Page on which Introduced</u>	<u>Dimensions</u>	<u>Definition</u>
<u>C. Subscripts and Superscripts</u>			
( ) <sub>d</sub>	34	-	Inert diluent specie.
( ) <sub>f</sub>	82	-	The fuel specie.
( ) <sub>i</sub>	7	-	The i'th chemical specie.
( ) <sub>o</sub>	88	-	The oxidizer specie.
( ) <sub>p</sub>	26	-	Product specie.
( ) <sub>I</sub>	29 and 48	-	Condition at the cold boundary.
( ) <sub>II</sub>	48	-	Condition at the hot boundary.
( ) <sup>N</sup>	73	-	The N'th Approximation to the indicated function.

## I. INTRODUCTION

The analytic treatment of gaseous flow systems with chemical reaction poses many new problems and greatly increases the complexity of the formulation and solution of the flow field. Although the consideration of flow fields with chemical reaction is not a recent innovation, Mallard and Le Chatelier<sup>(1)\*</sup> having treated the one-dimensional flame in 1883, the complexity of the problems and the relatively small effort expended in this field have conspired to limit the current state of knowledge to a rather primitive state. Only the simplest physical problems, reduced to yet simpler conceptual models, have been successfully attacked and the correlation of the analytic solutions with experimental data is generally not in good quantitative agreement. In connection with related experimental studies, however, the analytic studies have been of considerable value in determining the relative importance of various mechanisms postulated for reacting flow systems; furthermore, the qualitative trends indicated by analysis have usually been substantiated by experimental studies.

The large majority of analytic studies in "aerothermochemistry"<sup>(2)</sup> have been concerned with either of two problems: (1) the structure of simple one-dimensional flame fronts and detonation waves<sup>(3, 4, 5)</sup>, and (2) the influence of a flame front, treated as a surface of discontinuity, upon the flow field<sup>(6, 7)</sup>. Studies of these problems have yielded much useful information. However, many technically important problems

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\* Superscript numbers enclosed by parenthesis refer to the references; cf. pp. 150 - 155.

exist in which the essential physical phenomena cannot be approximated by either a plane one-dimensional flame or a surface of discontinuity in the flow field. For example, the stabilization limits (blowoff and flashback velocities) for a bluff body flame holder could be calculated in general only by considering a viscous two-dimensional or three-dimensional flow field with chemical reaction. As another example, flame front oscillations and turbulence would normally require the consideration of a non-steady two-dimensional or three-dimensional flow field with chemical reaction. Both of these problems appear to be intractable in view of the present state of knowledge in aerothermochemistry.

However, as pointed out by Marble and Adamson<sup>(8)</sup>, an entire class of technically important problems, namely those which can be treated using the classic Prandtl boundary layer assumptions, can be successfully attacked with the present state of knowledge. Problems falling within this class include, (1) the thermal quenching of a reacting gaseous mixture by a cool wall, briefly discussed by von Kármán and Millan<sup>(9)</sup>, (2) the thermal ignition of a combustible gaseous mixture by a heated wall, (3) combustion processes in free jets and combustion under conditions of mixing between two gaseous streams, (4) dissociation and recombination in a hypersonic boundary layer, and (5) the erosive burning of a solid propellant grain. Relatively little effort has been expended upon this technically important class of problems.

Marble and Adamson<sup>(8)</sup> considered problem (3) above; in particular they considered the case of a first-order chemical reaction occurring in a laminar mixing region having a velocity ratio of unity. An

equivalent, and almost identical, analysis of this problem has also been given by Pai<sup>(10)</sup>.

In the present study, the fruitful approach of Marble and Adamson is utilized. Their work is generalized to include second-order and third-order reactions as well as the first-order reaction and is extended to mixing regions with arbitrary velocity ratios and to combustion within the laminar boundary layer of a constant temperature flat plate. For the case where the Prandtl and Schmidt numbers are equal, the determination of a similarity function relating the specie concentrations to the local temperature greatly simplifies the analysis and leads to a general analytic solution for the N'th approximation to the temperature and concentration profiles in a reacting boundary layer type region. The similarity function is shown to be equal to the dimensionless streamwise velocity when the Prandtl and Schmidt numbers are both equal to unity.

The application of the similarity technique to one-dimensional flow fields is briefly discussed in Appendix E. Combustion in the laminar boundary layer with arbitrary wall temperature distribution is considered in Appendix F and chemical reaction in the hypersonic laminar boundary layer is briefly discussed in Appendix G.

## II. THE GOVERNING EQUATIONS OF CHANGE FOR ONE-DIMENSIONAL AND BOUNDARY LAYER TYPE FLOWING GASEOUS SYSTEMS WITH CHEMICAL REACTION

### A. General Equations of Change

The physical description of nonequilibrium systems such as flowing gases with chemical reaction is in the province of nonequilibrium statistical mechanics or modern kinetic theory<sup>(11, 12)</sup>. By virtue of rather recent developments in kinetic theory, the properties of a nonequilibrium dilute gas mixture may be adequately described by the set of distribution functions, one for each component of the mixture, which is obtained by the solution of a corresponding set of Boltzmann integro-differential equations. The fundamental Boltzmann equation may be derived from a physical and intuitive viewpoint<sup>(13, 14)</sup> which, though simple, unfortunately presents some logical difficulties; the equation may also be rigorously derived from the firm ground of the Liouville theorem of statistical mechanics<sup>(15, 16)</sup>. The Boltzmann equation is valid only at densities sufficiently low that the effect of collisions involving more than two molecules is negligible. This and the additional condition that the gas mixture behaves as a continuum (the mean free path of the gas molecules being short compared with all the macroscopic dimensions of the system) are certainly valid in the case of combustion in flowing gaseous systems at normal (near atmospheric) pressures.

The fundamental equations of change - continuity, momentum and energy balance - can be derived from the Boltzmann equation without actually determining the form of the distribution function<sup>(17)</sup>. Expressions for the fundamental equations of change for a flowing gaseous system

with chemical reaction are presented later in this section. However, certain functions, called the flux vectors, which involve the distribution functions appear in the expressions for the fundamental equations of change; the Boltzmann equation must thus be solved in order to evaluate the flux vectors.

In view of the complexity of the Boltzmann equation, it is not surprising that an exact solution has not been obtained and that considerable effort has been expended upon obtaining approximate solutions. The perturbation technique of Enskog, which is a modification of a method due to Hilbert, is the most widely used method of approximation. This technique involves a perturbation about the equilibrium state (the "zeroth-order" solution which corresponds to the Eulerian equations of motion) and is thus valid only when the distribution function at any point in the gas is only slightly different from a Maxwellian distribution. The first-order perturbation leads to the Navier-Stokes equations which apply to systems, such as are considered in this study, in which the gradients in physical properties are small in the sense that they do not change appreciably in a distance of a mean free path; phenomena such as shock and detonation waves cannot properly be treated by this order of approximation. The second-order perturbation leads to the Burnett equations which were formerly thought to be applicable to phenomena such as shock and detonation waves. Apparently, such is not the case<sup>(18)</sup>, however, and there is now considerable doubt as to the validity of the Burnett equations due to questions concerning the convergence of Enskog's series, causality, and the fact that proper statistical mechan-



ical modifications were not included<sup>(19)</sup>. Fortunately, the recent contribution by Grad<sup>(20)</sup> of a new method of solving the Boltzmann equation justifies the first approximation of Enskog with which we will be concerned.

Enskog's first perturbation leads to expressions for the flux vectors in terms of a set of integral equations\*. These equations explicitly involve the dynamics of a molecular encounter and hence the intermolecular force law. Even within the restrictions imposed by the assumptions previously noted, the accuracy of the calculation of the flux vectors and of the associated transport properties is thus related to the validity of the intermolecular force law utilized. Solutions to the integral equations, in terms of the properties of the molecular model employed, have been obtained by two equivalent methods. Chapman and Cowling<sup>(21)</sup> expanded the unknown scalar functions in an infinite series of Sonine polynomials; these polynomials are related to the associated Laguerre polynomials<sup>(22)</sup>. The flux vectors are then expressed in terms of ratios of infinite determinants. Curtiss and Hirschfelder<sup>(23)</sup> utilized a finite series of Sonine polynomials and employed a variational procedure in determining the coefficients of the expansion. The results of the latter work will be employed in this study. Expressions for the flux vectors in terms of the transport property coefficients are presented in Section II B; expressions for the transport property coefficients for a simple

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\* One additional assumption is made in the derivation of these integral equations: classical mechanics is employed. This restriction is unimportant in the present case and in all applications except where light gases are treated at very low temperatures.

molecular model, the Maxwellian molecule, are presented in Section II C.

With the above brief discussion for background, the general equations of change which include the effects of chemical reaction and molecular internal degrees of freedom will now be presented in the form derived by Hirschfelder, Curtiss and Bird<sup>(24)</sup>.

### 1. Continuity of Chemical Species

The equations for the continuity of the i'th chemical specie is\*,

$$\frac{\partial n_i}{\partial t} + \nabla \cdot [n_i (\vec{c}_0 + \vec{c}_i)] = \kappa_i \quad (1)$$

For a system consisting of N distinct chemical species, N such equations may be written; however, as will be discussed later, only N-1 of these equations are independent or necessary. The term  $\kappa_i$  represents a source strength due to the production of molecules of the i'th chemical specie; an expression for this term as a function of the thermodynamic variables and the parameters of chemical kinetics is presented in Section II D.

### 2. Conservation of Mass

In the absence of sources or sinks for mass, the overall relation for the conservation of mass may be obtained from equation 1 by multiplying through by  $m_i$ , summing over  $i$  and noting that  $\sum_i n_i m_i = \rho$  by definition and that  $\sum_i m_i n_i \vec{c}_i = \sum_i m_i \kappa_i = 0$  from mass conservation considerations<sup>(25)</sup>.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{c}_0 = 0 \quad (2)$$

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\* Refer to List of Symbols, pages x-xix, for definitions of the various symbols used.

### 3. Conservation of Momentum

In general there will be four equations for the conservation of momentum; one equation is required for each of the three translational degrees of freedom and a fourth equation, not generally considered, is strictly required for the conservation of angular momentum. If the molecules are smooth spheres, however, there is no mechanism for an interchange of the angular momentum associated with the rotation of the molecules with the angular momentum present in the form of the macroscopic motion of the gas. The impossibility of interchange of the angular momentum in the case of smooth spherical molecules negates the necessity of including the equation for the conservation of angular momentum. If the molecules are not smooth spheres, however, the equation for the conservation of angular momentum should be included as the interchange of angular momentum will introduce some modifications to the transport properties<sup>(26)</sup>.

Only smooth spherical molecules, represented by the Maxwellian molecular model (Section IIC), will be considered in the present paper. The equation for the conservation of angular momentum will thus be omitted.

The three scalar equations for the conservation of translational momenta may be expressed by the following vector equation:

$$\frac{D\vec{c}_0}{Dt} = \frac{\partial \vec{c}_0}{\partial t} + \vec{c}_0 \cdot \nabla \vec{c}_0 = -\frac{1}{\rho} \nabla \cdot \underline{\underline{P}} + \frac{1}{\rho} \sum_x n_x \vec{K}_x \quad (3)$$

The symbol  $\underline{\underline{P}}$  represents the pressure tensor, to be discussed in Section IIB, and  $\vec{K}_x$  is the force vector in dynes per molecule acting

on molecules of the i'th chemical specie due to an external field. The operator  $\frac{D}{Dt}$  is the Eulerian derivative,  $\frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{c}_0 \cdot \nabla$

#### 4. Conservation of Energy

The following form of the energy equation is valid for polyatomic as well as monatomic molecules and includes the effects of chemical reaction:

$$\rho \frac{Dc_v T}{Dt} = \rho \left[ \frac{\partial c_v T}{\partial t} + \vec{c}_0 \cdot \nabla c_v T \right] = -\nabla \cdot \vec{q} - \underline{p} : \nabla \vec{c}_0 + \sum_i n_i (\vec{c}_i \cdot \vec{X}_i) - \sum_i m_i K_i \hat{U}_i + \sum_i \hat{U}_i \nabla \cdot \vec{j}_i \quad (4)$$

The vector  $\vec{q}$  is the heat flux vector,  $\vec{j}_i$  is the mass flux vector for the i'th chemical specie, and  $\hat{U}_i$  is the total (thermodynamic plus chemical) internal energy per gram of the i'th chemical specie. The quantity  $c_v$  is the average heat capacity per gram of the mixture at constant volume. Thus,

$$c_v = \frac{1}{\rho} \sum_i n_i m_i \left( \frac{\partial \hat{U}_i}{\partial T} \right)_v = \frac{1}{\rho} \sum_i n_i m_i c_{v_i} \quad (5)$$

The heat and mass flux vectors are discussed in Section II B.

#### 5. Equation of State

Only five of the usual six hydrodynamic equations have been listed above. The remaining equation is that of thermodynamic state. It will be assumed that each component of the gas mixture obeys the thermodynamic equation of state of a perfect gas. Thus,

$$p_i = n_i kT$$

Furthermore, the validity of Dalton's law (the law of additivity of pressures at constant volume and temperature) will be assumed for the gas mixture. Then,

$$p = \sum_i p_i = n k T$$

or, in more convenient form,

$$p = \rho \frac{R}{M} T \quad (6)$$

where  $R$  is the universal gas constant ( $8.314 \times 10^7$  ergs/ $^{\circ}$ K/g-mole) and  $M$  is the equivalent molecular weight of the gas mixture; the corresponding units of pressure are dynes/cm<sup>2</sup>.

Expressions for the three flux vectors and for the chemical specie source strength due to chemical reaction are presented in the following sections in terms of the ordinary hydrodynamic and thermodynamic variables. They may thus be considered to be known quantities in the equations of change presented in the present section. The desired description of the reacting flow system is then given upon obtaining solutions for the unknown dependent variables in terms of the independent variables of time and the three space coordinates. The unknown dependent variables are the usual six variables of hydrodynamics - the three velocity components and the three thermodynamic variables of state (pressure, density and temperature) - plus the variable of chemical concentration for each of the species in the mixture. The latter variable may conveniently be expressed as a weight fraction. Since the sum of the weight fractions must be identically unity, only  $N-1$  equations for the continuity of chemical specie, equation 1, will be required if  $N$  is

the total number of distinct chemical species in the flow system. The set of equations is thus determinant as there are  $N + 6$  unknowns and an equal number of independent equations.

## B. The Flux Vectors

Under nonequilibrium conditions, gradients exist in one or more of the macroscopic physical properties of the system: composition, mass average velocity, and temperature. These gradients give rise respectively to the molecular transport of mass by diffusion, of momentum by the action of viscous and pressure forces, and of kinetic energy by the transfer of heat. The flux vectors which express these molecular transports are responsible for the irreversibility of the process or flow field under consideration. Expressions for the flux vectors of a binary mixture have been derived by Chapman and Cowling<sup>(11)</sup>; extension to the case of a general multi-component mixture has been made by Curtiss and Hirschfelder<sup>(23)</sup>. The following summary is based on the latter work.

### 1. The Mass Flux Vector and the Diffusion Velocity

The mass flux vector for the rate of molecular transport of the  $i$ 'th chemical specie is given by,

$$\vec{j}_i = n_i m_i \vec{c}_i \quad (7)$$

where the diffusion velocity  $\vec{c}_i$  is given by the expression,

$$\vec{c}_i = \left( \frac{n^2}{n_i g} \right) \sum_{j \neq i} m_j D_{ij} \vec{d}_j - \left( \frac{D_i^T}{n_i m_i} \right) \nabla \cdot \ln_e T \quad (8)$$

and the vector  $\vec{d}_j$  is expressed as,

$$\vec{d}_j = \nabla \left( \frac{n_j}{n} \right) + \left( \frac{n_j}{n} - \frac{n_j m_j}{\rho} \right) \nabla \cdot \ln_e \rho - \left( \frac{n_j m_j}{\rho^2} \right) \left[ \frac{\rho}{m_j} \vec{X}_j - \sum_l n_l \vec{X}_l \right] \quad (9)$$

The terms  $D_{\lambda j}$  and  $D_{\lambda}^T$  are the multicomponent diffusion coefficients and the multicomponent thermal diffusion coefficients, respectively\*. The multicomponent coefficients depend upon the physical properties, mass and law of interaction at collision, of the molecules of each of the chemical species present in the gas mixture and on the local composition and thermodynamic state. Expressions for these coefficients are given by Hirschfelder and his collaborators<sup>(28)</sup> in terms of the expansion coefficients of the finite series of Sonine polynomials used in their variational technique. The resulting expressions are very complex. Fortunately, by virtue of the simple molecular model which will be introduced in Section IIC, multicomponent diffusion and thermal diffusion coefficients will not be required in the analysis of this paper; therefore, they will not be considered hereafter. If desired, reference may be made to the excellent work of Hirschfelder, Curtiss and Bird, noted above, for a complete exposition of the current (1954) state of

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\* There is considerable variation among authors in the nomenclature and definition of the diffusion coefficients. Hirschfelder's nomenclature and definitions are used in this paper. See reference 27 for the relations between the diffusion coefficients used by Hirschfelder et al and those used by Chapman and Cowling.

knowledge with regard to multicomponent diffusion and thermal diffusion coefficients.

## 2. The Pressure Tensor

The pressure tensor represents the flux of momentum through the gas. The usual assumptions which are fundamental to the Navier-Stokes equations will be made; namely, that the gas medium is isotropic (no preferred direction) and that the normal and shear stresses are linear functions of the deformation velocities. The tensor is thus reduced to a symmetric second-order tensor whose diagonal elements are normal stresses and whose non-diagonal elements are shear stresses, the stresses being those measured by a suitable instrument moving with the stream velocity. For a dilute gas, the pressure tensor may be expressed as follows,

$$\underline{\underline{P}} = p \underline{\underline{U}} - 2\mu \underline{\underline{S}} - \eta \underline{\underline{U}} \nabla \cdot \vec{c}_0 \quad (10)$$

The unit tensor  $\underline{\underline{U}}$  and the rate of shear tensor  $\underline{\underline{S}}$  are given by,

$$\underline{\underline{U}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and

$$\underline{\underline{S}} = (S_{\alpha\beta})$$

where the components are as follows:

$$S_{\alpha\beta} = \frac{1}{2} \left[ \frac{\partial c_{0\beta}}{\partial x_{0\alpha}} + \frac{\partial c_{0\alpha}}{\partial x_{0\beta}} \right] - \frac{1}{3} \delta_{\alpha\beta} \nabla \cdot \vec{c}_0 \quad (11)$$



In equations 10 and 11,  $p$  is the equilibrium hydrostatic pressure (e. g., the local static pressure which would exist in the absence of velocity gradients) and  $\mu$  and  $\eta$  are the coefficients of shear and bulk viscosity respectively;  $\delta_{\alpha\beta}$  is the Kronecker delta, equal to unity when  $\alpha$  equals  $\beta$  and equal to zero when  $\alpha$  is not equal to  $\beta$ .

The coefficient of bulk viscosity (sometimes called the coefficient of dilatation viscosity) is closely related to the "relaxation time", a characteristic time required for the transfer of energy from the translational to the internal degrees of freedom. The bulk viscosity coefficient is zero for a dilute monatomic gas and is small, though non-zero, for a dilute polyatomic gas. Unless this coefficient vanishes, a spherically symmetrical expansion or contraction will give rise to a pressure different from the pressure of a gas at rest under the same conditions of density and temperature<sup>(29)</sup>. To avoid this complication, and in view of the lack of more complete information on the value of the bulk viscosity coefficient for polyatomic molecules, the validity of the classic Stoke's hypothesis of a zero bulk viscosity coefficient will be assumed; this assumption leads to results which are in good agreement with experimental measurements.

With the assumption of zero bulk viscosity, equations 10 and 11 can be combined to yield the following expressions for the diagonal and non-diagonal elements respectively of the symmetric pressure tensor:

$$\begin{aligned}
 P_{\alpha\alpha} &= p + \frac{2}{3} \mu \nabla \cdot \vec{C}_0 - 2\mu \frac{\partial C_{0\alpha}}{\partial x_{0\alpha}} \\
 P_{\alpha\beta} &= P_{\beta\alpha} = -\mu \left[ \frac{\partial C_{0\alpha}}{\partial x_{0\beta}} + \frac{\partial C_{0\beta}}{\partial x_{0\alpha}} \right] \quad ; \quad \alpha \neq \beta
 \end{aligned}
 \tag{12}$$

Upon operating on equation 12 with the appropriate rules for the manipulation of dyadics and tensors<sup>(30)</sup>, the following relations are obtained for the scalar product appearing in the energy equation and for the  $\alpha$ -component of the vector product appearing in the momentum equation:

$$\underline{\underline{P}} : \nabla \vec{C}_0 = \sum_{\alpha} \sum_{\beta} P_{\alpha\beta} \frac{\partial C_{0\alpha}}{\partial X_{0\beta}}$$

$$(\nabla \cdot \underline{\underline{P}})_{\alpha} = \sum_{\beta=1}^3 \frac{\partial P_{\alpha\beta}}{\partial X_{0\beta}}$$

Expansion of the above expressions yields the following relations

$$\begin{aligned} \underline{\underline{P}} : \nabla \vec{C}_0 &= \rho \nabla \cdot \vec{C}_0 - \mu \Phi \\ (\nabla \cdot \underline{\underline{P}})_{\alpha} &= \frac{\partial \rho}{\partial X_{0\alpha}} - \frac{\partial}{\partial X_{0\alpha}} \left[ \mu \left( 2 \frac{\partial C_{0\alpha}}{\partial X_{0\alpha}} - \frac{2}{3} \nabla \cdot \vec{C}_0 \right) \right] \\ &\quad - \sum_{\beta \neq \alpha} \frac{\partial}{\partial X_{0\beta}} \left[ \mu \left( \frac{\partial C_{0\alpha}}{\partial X_{0\beta}} + \frac{\partial C_{0\beta}}{\partial X_{0\alpha}} \right) \right] \end{aligned} \quad (13)$$

where  $\Phi$  contains the terms due to viscous dissipation<sup>(31, 32)</sup> and is given by,

$$\begin{aligned} \Phi &= 2 \left[ \left( \frac{\partial u_0}{\partial x_0} \right)^2 + \left( \frac{\partial v_0}{\partial y_0} \right)^2 + \left( \frac{\partial w_0}{\partial z_0} \right)^2 \right] \\ &\quad + \left( \frac{\partial v_0}{\partial x_0} + \frac{\partial u_0}{\partial y_0} \right)^2 + \left( \frac{\partial w_0}{\partial y_0} + \frac{\partial v_0}{\partial z_0} \right)^2 \\ &\quad + \left( \frac{\partial u_0}{\partial z_0} + \frac{\partial w_0}{\partial x_0} \right)^2 - \frac{2}{3} \left( \frac{\partial u_0}{\partial x_0} + \frac{\partial v_0}{\partial y_0} + \frac{\partial w_0}{\partial z_0} \right)^2 \end{aligned} \quad (14)$$

### 3. The Heat Flux Vector

The heat flux vector is given by the following expression:

$$\vec{q} = -\lambda \nabla T + \sum_i s_i \hat{h}_i \vec{c}_i + \frac{kT}{n} \sum_{i,j} \frac{n_j D_{ij}^T}{m_i D_{ij}} [\vec{c}_i - \vec{c}_j] \quad (15)$$

In the above,  $D_{ij}$  is the binary diffusion coefficient and  $\hat{h}_i$  is the total enthalpy (thermodynamic plus chemical) per gram of the i'th chemical specie. The terms on the right hand side of equation 15 are the rate of heat transfer by thermal conduction, ordinary diffusion, and thermal diffusion respectively.

It should be noted that the transfer of energy by radiation has not been included in the above expression for the heat flux vector. At the combustion pressures considered in the present paper, near atmospheric, the ratio of the energy transferred by radiation to the total energy transferred is very small. In view of this fact, the exploratory nature of the present investigation does not warrant the inclusion of this additional and cumbersome burden. A discussion of energy transfer by radiation and its influence upon the heat flux vector is given by Hirschfelder et al<sup>(33)</sup>; the influence of radiation upon flame propagation is treated by Gaydon<sup>(34)</sup> and by Magee<sup>(35)</sup>.

### C. Transport Properties for a Simple Molecular Model

It should be obvious from a cursory review of the expressions for the equations of change and for the flux vectors presented in the

preceding sections, that some rather drastic simplifications must be made if solutions are to be obtained. Simplifying assumptions with regard to the nature of the flow field will be made in Section IIE; in the present section assumptions will be made with regard to the molecular characteristics which determine the transport properties. The objective, of course, is to select a molecular model which is reasonably realistic and yet leads to simple expressions for the transport properties; furthermore, the model should be logically compatible with the assumptions which will later prove to be essential in the analysis to be presented. In particular, it is desirable that the Prandtl number, the Schmidt number, and the product of dynamic viscosity and density should be constants for the molecular model chosen.

Even if all species present in a gas mixture individually have simple expressions for the transport properties, the corresponding expressions for the transport properties of the gas mixture may still be very complex<sup>(28)</sup>. For example, the most elementary system in which chemical reactions can be considered, the binary system, will probably be mathematically intractable (at least in the absence of large digital computing machines) even if the transport coefficients of each component are simple. It follows that one desirable condition with regard to mathematical tractability is that the transport coefficients of the various components of a gas mixture be not only individually simple, but be equal.

One is thus driven to the realization that the most effective simplification that can be made with respect to the transport properties,

is the assumption of a gas mixture consisting of mechanically similar molecules. In this simple case the molecules of the various chemical species are of the same mass and obey the same law of interaction at encounter; the equivalence of molecular mass implies that the number of molecules in the gas mixture is not changed by chemical reaction. Note, however, that the molecules of different species may still differ in chemical reactivity. The coefficients of thermal conductivity and of viscosity for the mixture are then the same as if the molecules were identical in all respects (e. g., the mixture coefficients reduce identically to those of a pure component), the coefficient of thermal diffusion vanishes, and the coefficient of ordinary diffusion reduces to the coefficient of self-diffusion of a simple one-component gas<sup>(36)</sup>.

The mechanically similar molecules will be assumed to be Maxwellian (e. g., a molecule is assumed to be a point center of force repelling the nearest neighboring molecule with a force of magnitude  $\alpha r^{-5}$  where  $\alpha$  is the force constant of proportionality and  $r$  is the distance between the two molecules). Maxwellian molecules are reasonably fair approximations to reality, particularly at the high temperatures of interest in combustion where the contributions due to the repulsive forces are far more important than those due to attractive forces. Furthermore, the expressions for the transport properties of Maxwellian molecules are much simpler than are those for the more realistic molecular models such as that of Lennard-Jones.

Expressions for the transport properties of a one-component gas whose molecules are represented by point centers of force repelling

with a force of magnitude  $\propto r^{-2}$  are given by Hirschfelder, Curtiss and Bird<sup>(37)</sup>; proceeding from these general expressions, the transport properties for a gas mixture composed of mechanically similar Maxwellian molecules,  $\nu = 5$ , can be shown to be of the following form:

$$\begin{aligned} \mu &= \frac{k}{1.848 \pi} \sqrt{\frac{m}{\alpha}} \quad T \\ \mathcal{D} &= \frac{k}{1.192 \pi} \sqrt{\frac{m}{\alpha}} \quad \frac{T}{\rho} \\ \lambda^{\circ} &= \frac{5}{2} \mu C_v \end{aligned} \quad (16)$$

In the above, the expressions for the coefficients of viscosity and of diffusion are valid for polyatomic as well as monatomic gases; the expression for the thermal conductivity, however, is valid only for monatomic gases. This latter restriction is due to the presence of the internal degrees of freedom in polyatomic molecules and the consequent effect resulting from the time lag in the transfer of energy from the translational to the internal degrees of freedom. Since the internal degrees of freedom do not participate in the transfer of mass or of translational momentum, their presence does not affect the expressions for the diffusion and viscosity coefficients.

The Eucken correction<sup>(38)</sup> for the thermal conductivity of polyatomic molecules will be employed\*. With this approximation, the

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\* Because of the difficulty of transferring energy from the translational to the internal degrees of freedom at room temperatures, the Eucken correction does not fit experimental data accurately at these temperatures. At the higher temperatures of interest in combustion studies, however, the difficulty of transferring energy is much less and the Eucken correction should be applicable.

coefficient of thermal conductivity for polyatomic molecules is given by

$$\lambda = \mu \left[ c_p + \frac{5}{4} \frac{R}{M} \right] \quad (17)$$

where  $R$  is the universal gas constant and  $M$  is the equivalent molecular weight of the gas mixture.

Simple expressions for the Prandtl and Schmidt numbers of a mixture of mechanically similar Maxwellian molecules can be obtained from equations 16 and 17 with the following results:

$$\left. \begin{aligned} P_r &\equiv \frac{c_p \mu}{\lambda} = \frac{c_p}{\left[ c_p + \frac{5}{4} \frac{R}{M} \right]} \\ S_c &\equiv \frac{\mu}{\rho \lambda} = \frac{1.192}{1.848} = 0.646 \end{aligned} \right\} \quad (18)$$

The assumption is now made that the components of the gas mixture are all calorically perfect; the specific heats are thus independent of temperature. If, in addition, it is assumed that the specific heats of the various chemical species are equal ( $c_{p_i} = c_{p_j} = c_p$ ;  $c_{v_i} = c_{v_j} = c_v$ ), then the specific heats of the mixture will also be independent of the chemical composition and will, by virtue of the above, be constant. Under these conditions, the Prandtl number, as well as the Schmidt number, is constant. Furthermore, since the assumption that the mixture obeys the equation of state of a perfect gas has already been made (Section II A ), then  $\rho \sim T^{-1}$ ; thus from equation 16:

$$\mu \rho = \mu_{\pm} \rho_{\pm} = \text{constant} \quad (19)$$

This result will be exploited in Section IIF through utilization of the Howarth transformation.

#### D. Rate of Production of Chemical Species

The weight rate of production of chemical species enters explicitly into the expressions for the continuity of chemical specie and for the conservation of energy. The rate of production is dependent upon the concentrations of all of the reacting species and upon the specific reaction-rate coefficient. The form of the rate law which is appropriate is dependent upon the type of reaction: opposed or unopposed, single or multi-stepped. The assumption, which is not rigorously justifiable, is made that the reaction-rate laws of classical chemical kinetics which were derived for stationary, isothermal systems are applicable to non-isothermal flowing systems. The argument is made that although the phenomenological description of the flowing, non-isothermal system is different than that of the stationary isothermal system, the conditions on the microscopic level which govern the rate of energetic collisions and consequently the rate of chemical reaction are essentially unchanged\*. Brief introductory treatments of the

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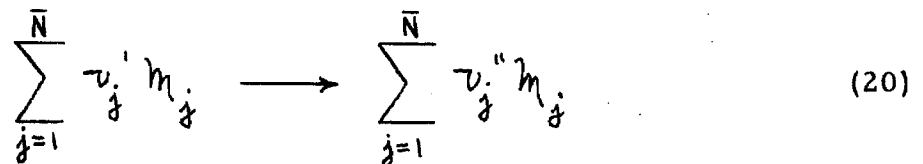
\* This argument is not valid in the treatment of physical phenomena, such as detonation waves, in which the temperature gradient is unusually large. Note, however, that the assumption of small gradients in the physical properties, in the sense that they do not change appreciably in the distance of a molecular mean free path, has already been made in Section IIA as an essential restriction on the validity of the Navier-Stokes equations. Thus the above assumption as to the validity of classical chemical kinetics does not give rise to additional restrictions on the type of systems which can be treated with the present analytical machinery, but rather is consistent with the previous development of the expressions for the flux vectors.



reaction-rate laws are given by Penner<sup>(39)</sup> and by Taylor<sup>(40)</sup>. More extensive treatments of chemical kinetics are presented in references 41, 42 and 43.

Only one-step chemical reactions in which the forward reaction is dominant and the backward reaction is consequently completely negligible will be considered in the main body of this paper\*. In exploratory studies such as the present, such a simple "global" reaction is an acceptable model for the complex multi-stepped chemical reactions which actually occur in technical exothermic combustion processes<sup>(44)</sup>. Advanced analysis of a quantitative nature will of course require a more sophisticated approach which considers multi-stepped and opposed reactions.

The one-step forward reaction of arbitrary complexity may be represented by the equation



where the  $v_j^{\prime}$  and  $v_j^{\prime\prime}$  are the stoichiometric coefficients for the reactants and products respectively;  $m_j$  stands for the j'th chemical specie and  $\bar{N}$  is the total number of different chemical species which take part in the reaction. The reaction represented in equation 20 is

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\* A simple one-step opposed reaction is considered in Appendix G in the course of a brief discussion and analysis of an important technical problem - dissociation and recombination in the hypersonic boundary layer.

said to have an overall order,  $m^*$ , equal to the summation of the coefficients of the reactants,  $m^* = \sum_{j=1}^{\bar{N}} \nu_j'$ .

According to the law of mass action, the net mass rate of production per unit volume of the  $i$ 'th chemical specie,  $m_i R_i$ , due to the chemical reaction represented by equation 20 is given by the expression:

$$m_i R_i = M_i (\nu_i'' - \nu_i') k_f \prod_{j=1}^{\bar{N}} \left( \frac{S K_j}{M_j} \right)^{\nu_j'} \quad (21)$$

The proportionality factor  $k_f$  is called the specific reaction-rate coefficient;  $K_j$  and  $M_j$  are the weight fraction and molecular weight of specie  $j$  respectively. According to the classical Arrhenius equation<sup>(45)</sup>, which will be utilized in the present study, the specific reaction-rate coefficient is given by,

$$k_f = b \exp[-E/RT] \quad (22)$$

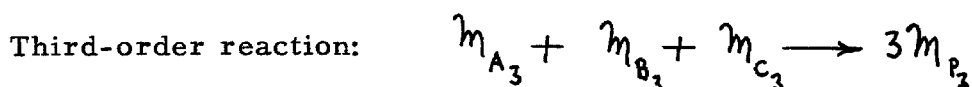
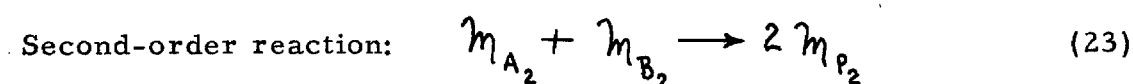
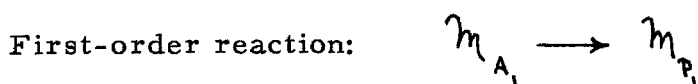
where  $b$  is the so-called frequency factor\* and  $E$  is the activation energy (per gram mole of stoichiometric mixture) for the reaction.

\* The so-called frequency factor actually has the dimensions of frequency only for the particular case of a first-order reaction. For a reaction of order  $m^*$ , the dimensions of the "frequency factor" are actually as follows:

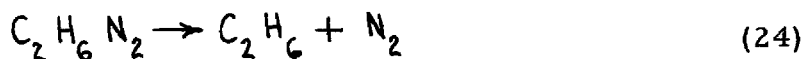
$$(\text{moles})^{1-m^*} (\text{cm}^3)^{m^*-1} (\text{sec})^{-1}. \text{ See reference 46 for a derivation}$$

of this dimensional expression. Note that from equation 22, the dimensions of the specific reaction-rate coefficient are identical with those of the so-called frequency factor.

In conformity with the assumption of Section IIC with regard to mechanically similar molecules, the reactions considered will be limited to those in which all chemical species involved have the same molecular weight; thus, the number of molecules present in the gas mixture will not be affected by the occurrence of chemical reaction. A simple first-order, a simple second-order, and a simple third-order reaction will be considered; the corresponding reactions are listed below:



The thermal decomposition of azomethane is an example of a complex chemical reaction which obeys first-order kinetics rate laws\*. This reaction, which will be considered as the basis for first-order kinetics calculations in certain of the following sections, has been discussed in considerable detail by Kassel<sup>(48, 49)</sup>, by Ramsperger<sup>(47, 50)</sup>, and by Rice and Ramsperger<sup>(51)</sup>. The principal reaction is given by the equation




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\* Ramsperger<sup>(47)</sup> experimentally determined that the decomposition of azomethane is essentially a first-order or unimolecular reaction at "high pressures" (e. g., at pressures of about 700 mm Hg., thus near the pressure level considered in the present paper) but rapidly degenerates to a fractional order reaction as the pressure decreases.

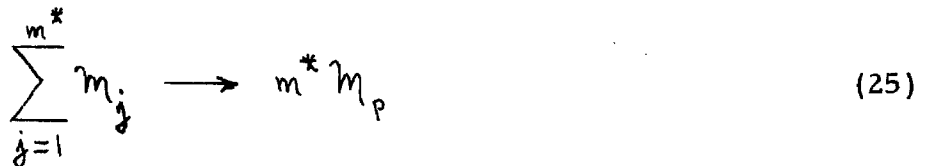
which indicates that one molecule of azomethane decomposes to yield one molecule of ethane and one molecule of nitrogen. However, there is a small amount of side reaction as indicated by the presence of about 1.7 % of unsaturated hydrocarbons in the reactant products; this side reaction will be neglected in the present paper. Note that in equation 24, the products are similar in molecular weight and may be treated as consisting of two molecules of a hypothetical chemical specie of molecular weight 29 having properties between those of  $C_2H_6$  and  $N_2$ . Other examples of complex reactions obeying first-order kinetics rate laws are the decomposition of  $N_2O_5$ , the thermal decomposition of certain hydrocarbons, and the decomposition of the azo compounds, azoisopropane, methyl isopropyl diimide and dimethyl triazene<sup>(52)</sup>.

Many chemical reactions of technological importance follow second-order kinetics. When the reaction is complex and follows this order of kinetics, it is probable that the rate-determining or "slow" step is a bimolecular process. The combustion of hydrocarbon fuels with air is generally thought to be governed by rate-controlling bimolecular processes obeying second-order kinetics. A simple one-step second-order reaction such as that of equation 23 may thus be taken as a reasonable though crude model for exploratory analytic investigations of air, hydrocarbon fuel combustion.

Third-order reactions may be classified into two groups: those in which all of the molecules involved enter into the chemical equation for the reaction, and those in which the third molecule is needed only to remove the excess heat of reaction and permit the two reacting

molecules to combine. Only four of the first group of reactions are known; each of these is second-order with respect to nitric oxide and first-order with respect to the other substance - oxygen, chlorine, bromine, or hydrogen. These reactions have been rather thoroughly studied, while reactions of the second group have not been thoroughly studied. Since none of the third-order reactions are of paramount interest in technical combustion processes, no numerical calculations for this order of reaction will be carried out. Inasmuch, however, as the analysis for third-order reactions can be carried through with no additional difficulty, the analysis will be presented in such a form as to be directly applicable to this order of reaction as well as to the more common first-order and second-order reactions.

Now if the order of reaction is denoted by the symbol  $m^*$ , and the product specie is denoted by the subscript  $p$ , then the reactions of equation 23 may be summarized in the single expression:



The corresponding general expression for the mass rate of production of a reactant specie per unit volume is obtained upon combining equations 21, 22, and 25:

$$m_i R_i = -M_i b \exp[-E/RT] \prod_{j=1}^{m^*} \left( \frac{S K_j}{M_j} \right) \quad (26)$$

From the equation of state, equation 6, it follows that  $S/M = P/RT$ .

Noting from the above equation that the mass rate of production of all reactant species is the same (since molecular weights and stoichiometric coefficients are equal), and defining  $w_{\sim}$  as the mass rate of removal of any given reactant specie per unit volume and per unit density, the following relation is obtained:

$$w_{\sim} \equiv -\frac{m_{\sim} K_{\sim}}{\rho} = b \left( \frac{P}{RT} \right)^{m^* - 1} \exp[-E/RT] \prod_{j=1}^{m^*} K_j \quad (27)$$

From equations 25 and 26 and the principle of the conservation of mass, it follows that the mass rate of production of the product specie per unit volume and per unit density is given by:

$$w_p \equiv -\frac{1}{\rho} \sum_{i=1}^{m^*} m_{\sim} K_{\sim} = m^* w_{\sim} \quad (28)$$

It will now be convenient to develop an expression for the sum  $\sum_{i=1}^N m_{\sim} K_{\sim} \hat{U}_{\sim}$  which occurs in the energy balance equation, equation 4, for the particular class of reactions represented by equation 25. Since  $\hat{U}_{\sim}$  is the total (thermodynamic plus chemical) internal energy of the i'th chemical specie,

$$\hat{U}_{\sim} = \Delta H_{f_{\sim}}^{\circ} + \int_{298.16}^T c_{v_{\sim}}(\tau) d\tau \quad (29)$$

where  $\Delta H_{f_{\sim}}^{\circ}$  is the standard heat of formation (per gram) of the i'th chemical specie at 298.16 degrees Kelvin. Using the assumption from Section IIC that  $c_{v_i} = c_{v_j} = c_v = \text{constant}$  it follows that:

$$\sum_{i=1}^{\bar{N}} m_i K_i \hat{U}_i = \sum_{i=1}^{\bar{N}} m_i K_i \Delta H_{f_i}^{\circ} + c_v (T-298.16) \sum_{i=1}^{\bar{N}} m_i K_i$$

However,  $\sum_{i=1}^{\bar{N}} m_i K_i$  is identically zero by virtue of the conservation of mass; thus,

$$\sum_{i=1}^{\bar{N}} m_i K_i \hat{U}_i = \sum_{i=1}^{\bar{N}} m_i K_i \Delta H_{f_i}^{\circ} \quad (30)$$

Equation 30 is a general expression valid for any reaction for which the assumption of constant specific heats is acceptable.

Now for the particular class of reactions represented by equation 25, the first  $\bar{N}-1$  terms of the above sum are concerned with the reactants and the last term is concerned with the product specie; thus from the above,

$$\left. \begin{aligned} m_i K_i &= -\rho w_r & ; & i < \bar{N} \\ m_i K_i &= \rho w_p & ; & i = \bar{N} \end{aligned} \right\} \quad (31)$$

where,

$$\bar{N} = m^* + 1$$

Combination of equations 28, 30, and 31 yields,

$$-\frac{1}{\rho c_p} \sum_{i=1}^{\bar{N}} m_i K_i \hat{U}_i = w_r \bar{\Delta H} \quad (32)$$

where:

$$c_p \bar{\Delta H} = \sum_{j=1}^{m^*} \Delta H_{f_j}^{\circ} - m^* \Delta H_{f_p}^{\circ} \quad (33)$$

is the excess of chemical energy which a combustible mixture containing one gram of each reactant specie and satisfying equation 25, has available for conversion to thermal energy;  $\Delta H_{f_j}^{\circ}$  and  $\Delta H_{f_p}^{\circ}$  are the standard heats of formation of the j'th reactant specie and the product specie respectively. Note that for an exothermic chemical reaction at constant pressure, the conversion of chemical to thermal energy satisfies the simple relation:

$$\overline{\Delta H} = m^* (T_f - T_I) \quad (34)$$

where  $T_f$  is the adiabatic flame temperature for a stoichiometric mixture which is initially, in the cold premixed state, at the temperature  $T_I$  of the combustible free stream. The previous assumption of constant specific heats is, of course, essential to the validity of equation 34.

#### E. Equations of Change for Combustion in One-Dimensional and Laminar Boundary Layer Type Flow Systems

The complexity of the expressions for the general equations of change (Section II A) and for the flux vectors (Section II B) demands that rather drastic simplifications be made before the analysis can proceed. Simplifying assumptions with regard to the molecular properties of the gas mixture were made in Section II C with the consequent results that:



$$\begin{aligned}
 m_i &= m = \text{constant} \\
 M_i &= M = \text{constant} \\
 c_{v_i} &= c_v = \text{constant} \\
 c_{p_i} &= c_p = c_v + \mathcal{R}/M = \text{constant} \\
 Pr &= c_p \mu / \lambda = \text{constant} \\
 Sc &= \mu / \rho \mathcal{D} = \text{constant} \\
 \mu \rho &= \mu_{\pm} \rho_{\pm} = \text{constant} \\
 \mathcal{D} &= \mathcal{D}_{ij} = \mathcal{D}_{ji} \\
 D_i^T &= 0 \text{ (thermal diffusivity vanishes)}
 \end{aligned}
 \tag{35}$$

Although these results serve to materially simplify the fundamental equations governing the reacting flow system, additional assumptions with regard to the nature of the flow field will now be made in order to obtain the least complex set of governing equations consistent with the class of flow systems to be considered in the analysis.

Three assumptions with regard to the flow field will be made: First, it will be assumed that all viscous regions and flame fronts are laminar; treatment of the turbulent case appears to be possible but much more complex and will not be considered in the present paper. Second, the absence of external forces acting on the gas molecules will be assumed. In practice this assumption requires that the flow velocity be sufficiently high so that the gravitational influences are negligible; furthermore, consideration of the interesting problem of the influence of magnetic and/or electric fields on the reacting (and possibly

ionized) gases is thus excluded. The third assumption is that of a constant pressure flow field. This implies that the radius of curvature of the streamlines is very large and that the free stream velocity is steady; the present analysis must thus be restricted to non-accelerating one-dimensional flows or to steady planar boundary layer type flows. The implication is also made that the pressure change through a laminar deflagration wave is negligibly small, an implication which is in accord with reality<sup>(53)</sup>. From the above,

- a.  $p = \text{constant}$
  - b.  $\vec{X}_\nu = 0$
  - c. Flow is laminar
- (36)

These three assumptions with respect to the nature of the flow field, when coupled with the results of Section IIC which are summarized in equation 35, result in a very great simplification of the expressions for the flux vectors and for the equations of change. Furthermore, they still permit the treatment of a class of technically important combustion problems - namely the planar boundary layer type of phenomena in which the variations in the physical properties of the flow system are much greater in a direction normal to the main flow than they are in the streamwise direction. The simpler class of one-dimensional systems may also be considered.

In the present section, equations 35 and 36 will be utilized in reducing the general expressions for the equations of change (Section II A) and the flux vectors (Section II B) to the simplified forms which serve as the basis for the analysis which is to follow.

1. Simplified Expressions for the Mass and Heat Flux Vectors

Combination of equations 8, 9, 35, and 36 yields the following simple expression for the diffusion velocity,

$$\vec{C}_i = \frac{n^2}{n_i \rho} \sum_{j \neq i} m_j \mathcal{D} \nabla (n_j/n)$$

noting that  $m_j = m$  (mechanically similar molecules),  $nm = \rho$  and introducing  $K_j = n_j/n$  as the weight fraction of specie j,

$$\vec{C}_i = \frac{\mathcal{D}}{K_i} \sum_{j \neq i} \nabla K_j$$

or, since  $\sum_j K_j = 1$  and  $\sum_{j \neq i} K_j = 1 - K_i$ ,

$$\vec{C}_i = -\frac{\mathcal{D}}{K_i} \nabla K_i \quad (37)$$

From the above and equations 7 and 35 the divergence of the mass flux vector may be expressed as,

$$\nabla \cdot \vec{j}_i = \nabla \cdot [-\rho \mathcal{D} \nabla K_i] = -\nabla \cdot \left[ \frac{\mu}{Sc} \nabla K_i \right] \quad (38)$$

In similar manner, the heat flux vector, equation 15 can be simplified to,

$$\vec{q} = -\left[ \lambda \nabla T + \frac{\mu}{Sc} \sum_i \hat{h}_i \nabla K_i \right] \quad (39)$$

Now since,

$$\hat{U}_i = \hat{h}_i - p/\rho \quad (40)$$

the following sum which appears in the energy balance relation, equation 4, may be simplified through the use of equations 38 through 40:

$$\begin{aligned}
 -\nabla \cdot \vec{q} + \sum_i \hat{c}_i \nabla \cdot \vec{j}_i &= \nabla \cdot \lambda \nabla T + \sum_i \nabla \cdot \left[ \frac{\mu}{S_c} \hat{h}_i \nabla K_i \right] \\
 &\quad - \sum_i \left[ (\hat{h}_i - \rho/\rho) \left( \nabla \cdot \frac{\mu}{S_c} \nabla K_i \right) \right] \\
 &= \nabla \cdot \lambda \nabla T + (\rho/\rho) \nabla \cdot \left[ \frac{\mu}{S_c} \nabla \sum_i K_i \right] \\
 &\quad + \frac{\mu}{S_c} \sum_i \left[ \nabla K_i \cdot \nabla \hat{h}_i \right]
 \end{aligned}$$

For a calorically perfect gas mixture with constant specific heats as previously assumed,  $\nabla \hat{h}_i = c_p \nabla T$ . Furthermore,  $\nabla \sum_i K_i = 0$ ; the following simple result is thus obtained:

$$-\nabla \cdot \vec{q} + \sum_i \hat{c}_i \nabla \cdot \vec{j}_i = \nabla \cdot \lambda \nabla T \tag{41}$$

## 2. The Equation for the Continuity of Chemical Specie

Upon multiplying equation 1 through by  $m = m_i$ , noting that  $m n_i = \rho K_i$ , and using equation 37, it is found that:

$$\frac{\partial(\rho K_i)}{\partial t} + \nabla \cdot \left[ \rho K_i \vec{c}_0 - \rho D \nabla K_i \right] = m_i K_i \equiv -w_i \rho$$

where  $w_i$  is the mass rate of removal (per unit volume and per unit density) of the i'th chemical specie from the system. Furthermore, since

$$\nabla \cdot \rho K_i \vec{c}_0 = K_i \nabla \cdot \rho \vec{c}_0 + \rho \vec{c}_0 \cdot \nabla K_i$$

and  $\rho \bar{D} = \mu / S_c$ , the above may also be written as,

$$\rho \left[ \frac{\partial K_i}{\partial t} + \vec{C}_0 \cdot \nabla K_i \right] + K_i \left[ \frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{C}_0 \right] - \nabla \cdot \left[ \frac{\mu}{S_c} \nabla K_i \right] = -w_i \rho$$

The coefficient of  $K_i$  is identically zero by virtue of the relation for the conservation of mass, equation 2. In the case of a chemical system reacting according to equation 25 and containing one inert diluent specie, the continuity of the  $m^* + 2$  chemical species may thus be accounted for by the following expressions:

$$\left. \begin{aligned} \text{a) } \frac{DK_i}{Dt} &= \frac{1}{S} \nabla \cdot \left( \frac{\mu}{S_c} \nabla K_i \right) - w_i \quad ; \quad i \neq p \\ \text{where: } w_i &= \begin{cases} w_i & i \leq m^* \\ 0 & i = d \end{cases} \\ \text{b) } K_p &= 1 - K_d - \sum_{j=1}^{m^*} K_j \end{aligned} \right\} \quad (42)$$

The subscript d refers to the inert diluent specie, the subscript p refers to the product specie, and the  $m^*$  values of i other than d and p refer to the  $m^*$  reactant species. Since the last term in equation 42a is related to the rate at which the i'th specie is being removed by chemical reaction, this term must be zero in the case of the inert specie. Equation 42b is simply a statement of the fact that the sum of the weight fractions must be unity.

### 3. The Energy Balance Equation

The left hand side of the energy balance relation, equation 4, may conveniently be expressed in terms of the constant pressure specific heat rather than in terms of the constant volume specific heat. For a perfect gas as has already been assumed,

$$c_v = c_p - p/\rho T$$

thus, noting that the assumption of constant specific heats has already been made,

$$\rho \frac{Dc_v T}{Dt} = \rho c_v \frac{DT}{Dt} = \rho c_p \frac{DT}{Dt} - \frac{p}{T} \frac{DT}{Dt}$$

The last Eulerian derivative in the above can be expressed in a more convenient form through the use of the equation for the conservation of mass in the form  $\frac{D\rho}{Dt} = -\rho \nabla \cdot \vec{c}_0$ , for then,

$$(p/T) \frac{DT}{Dt} = \frac{Dp}{Dt} - T \frac{\rho}{M} \frac{D\rho}{Dt} = \frac{Dp}{Dt} + p \nabla \cdot \vec{c}_0$$

and, finally,

$$\rho \frac{Dc_v T}{Dt} = \rho c_p \frac{DT}{Dt} - \frac{Dp}{Dt} - p \nabla \cdot \vec{c}_0 \quad (43)$$

Substitution of equations 13, 41, and 43 into equation 4 and the utilization of equations 35 and 36 yields the following expression for the energy balance relation:

$$\frac{DT}{Dt} = \frac{\mu}{\rho c_p} \Phi - \frac{1}{\rho c_p} \sum_{\lambda=1}^{\bar{N}} m_{\lambda} \kappa_{\lambda} \hat{U}_{\lambda} + \frac{1}{\rho} \nabla \cdot \left( \frac{\mu}{Pr} \nabla T \right)$$

In the exothermic combustion problems to be considered in the following sections, the ratio of thermal to kinetic energy is so high as to make

the viscous dissipation function  $\Phi$  in the above expression completely negligible\* ; thus  $\Phi$  will be set equal to zero. With the use of this approximation and the application of equations 32 and 34, the above relation reduces to the expression:

$$\frac{DT}{Dt} = \frac{1}{\rho} \nabla \cdot \left( \frac{\mu}{Pr} \nabla T \right) + m^* \omega_{\sim} (T_f - T_I) \quad (44)$$

An expression for  $\omega_{\sim}$  is given in equation 27,

#### 4. The Equation for the Conservation of Momentum

Upon substitution of equations 13 and 35 into equation 3, the following expression for the conservation of the  $\alpha$  -component of translational momentum is obtained for the case of a constant pressure flow field:

$$\begin{aligned} \frac{DC_{o\alpha}}{Dt} &= \frac{1}{\rho} \frac{\partial}{\partial x_{o\alpha}} \left[ \mu \left( 2 \frac{\partial C_{o\alpha}}{\partial x_{o\alpha}} - \frac{2}{3} \nabla \cdot \vec{C}_o \right) \right] \\ &+ \frac{1}{\rho} \sum_{\beta \neq \alpha} \frac{\partial}{\partial x_{o\beta}} \left[ \mu \left( \frac{\partial C_{o\alpha}}{\partial x_{o\beta}} + \frac{\partial C_{o\beta}}{\partial x_{o\alpha}} \right) \right] \end{aligned} \quad (45)$$

#### 5. Compilation of the Governing Equations for One-Dimensional Flow Systems

Although one-dimensional flow systems will not be treated in the

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\* An important technical problem, that of the chemical reaction in hypersonic boundary layers is briefly treated in Appendix G. In this high speed flow case, of course, the viscous dissipation is relatively large and must be included.

main body of the present paper, many of the analytic techniques used in the following sections are directly applicable to the simpler one-dimensional systems\*. The governing equations for one-dimensional flow systems will thus be summarized for future reference.

For simple one-dimensional flow systems, the differential operators which appear in the preceding equations take the following special forms:

$$\left. \begin{aligned} \frac{D}{Dt} &= \frac{\partial}{\partial t} + u_0 \frac{\partial}{\partial x_0} \\ \nabla \cdot \vec{A} &= \frac{\partial A_{x_0}}{\partial x_0} \\ \nabla B &= \frac{\partial B_{x_0}}{\partial x_0} \vec{i} \end{aligned} \right\} \quad (46)$$

The governing relations for one-dimensional flow systems with chemical reaction are obtained upon compiling equations 2, 6, and 27, and simplifying equations 42, 44, and 45 according to equation 46. The chemical reaction may follow first-order, second-order, or third-order kinetics, according to equation 25, and one inert diluent specie may be included. The gas mixture will thus consist of  $m^* + 2$  distinct chemical species:  $m^*$  reactant species, the product specie, and the inert diluent specie. Note that the following set of governing equations is valid only when the restrictions of equations 25, 35, and 36 are satisfied.

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\* The application of similarity techniques to one-dimensional, reacting flow systems is briefly discussed in Appendix E.



One-dimensional flow systems:

$$a) \quad \frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_0)}{\partial x_0} = 0$$

$$b) \quad \frac{\partial T}{\partial t} + u_0 \frac{\partial T}{\partial x_0} = \frac{1}{S} \frac{\partial}{\partial x_0} \left( \frac{\mu}{Pr} \frac{\partial T}{\partial x_0} \right) + m^* \omega_{\sim} (T_f - T_{\pm})$$

$$c) \quad \frac{\partial K_i}{\partial t} + u_0 \frac{\partial K_i}{\partial x_0} = \frac{1}{S} \frac{\partial}{\partial x_0} \left( \frac{\mu}{Sc} \frac{\partial K_i}{\partial x_0} \right) - \omega_i ; i \neq p$$

$$\text{where: } \omega_i = \begin{cases} \omega_{\sim} & i \leq m^* \\ 0 & i = d \end{cases}$$

(47)

$$d) \quad K_p = 1 - K_d - \sum_{j=1}^{m^*} K_j$$

$$e) \quad \omega_{\sim} = b \left( \frac{p}{RT} \right)^{m^*-1} \exp[-E/RT] \prod_{j=1}^{m^*} K_j$$

$$f) \quad S = \frac{\rho M}{RT}$$

Note that for the case of present interest, a one-dimensional constant pressure flow field, the momentum equation is not necessary. The  $m^* + 5$  unknowns (velocity, temperature, density, and the  $m^* + 2$  weight fractions) are completely specified by a simultaneous solution of the above  $m^* + 5$  independent governing relations.

6. Compilation of the Governing Equations for Planar, Laminar Boundary Layer Type Flow Systems

In assuming a constant pressure flow field in Section II E, it was noted that this assumption is valid even in the presence of chemical reaction since the pressure change through a laminar deflagration wave is negligibly small. Now, since there are no additional terms due to chemical reaction in the momentum relation, equation 45, and since the chemically induced pressure changes are negligible, it follows that the classic Prandtl boundary layer assumptions will be valid with regard to this equation. Thus the axial or streamwise momentum equation is simplified and the normal or lateral momentum equation simply indicates that the lateral pressure variation is negligible, an assumption which has already been made. The lateral momentum equation is thus deleted.

Since the relations for the conservation of mass, equation 2 and of thermodynamic state, equation 6, are also unaffected by chemical reaction, the application of the boundary layer assumptions in the presence of chemical reaction requires clarification only with regard to the continuity of chemical specie, equation 42, and with regard to the energy balance relation, equation 44. Each of these relations has a reaction term which is explicitly independent of the velocity or of any velocity derivatives. The order of magnitude comparison usually made in boundary layer theory may thus be accomplished without regard to the additional combustion terms; the normal boundary layer equations for energy balance and specie continuity, modified by a single chemical reaction term are then obtained. However, in making the classic boundary layer assumptions in the order of magnitude comparison, it

is assumed that the changes in the chemical concentration, temperature, and velocity in the streamwise direction are negligible in comparison to corresponding changes in the lateral or normal direction. The assumption is tacitly made, therefore, that the reaction induced changes in these variables follow this same pattern. The normal boundary layer equations for specie continuity and energy balance when modified by the addition of a reaction term are thus valid only in a region in which the chemically induced changes in temperature, concentration, and velocity are much greater in the lateral direction than in the streamwise direction. The consequent limitations in the applicability of the boundary layer equations to reacting flow systems, particularly in the case of the heated flat plate, will be brought out in later sections.

The governing relations for planar, laminar boundary layer type flow systems are obtained upon compiling equations 2, 6, and 27, and simplifying equations 42, 44, and 45 according to the classic Prandtl boundary layer assumptions (see reference 54 for detailed discussions of the Prandtl assumptions). The chemical reaction may follow first-order, second-order, or third-order kinetics. Note, however, that the following set of equations is valid only when the restrictions of equations 25, 35, and 36, and the fundamental restriction noted in the paragraph above are all satisfied.

Planar, laminar boundary layer type flow systems:

$$a) \quad \frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_0)}{\partial x_0} + \frac{\partial(\rho v_0)}{\partial y_0} = 0$$

$$b) \quad \frac{\partial u_0}{\partial t} + u_0 \frac{\partial u_0}{\partial x_0} + v_0 \frac{\partial u_0}{\partial y_0} = \frac{1}{\rho} \frac{\partial}{\partial y_0} \left( \mu \frac{\partial u_0}{\partial y_0} \right)$$

$$c) \quad \frac{\partial T}{\partial t} + u_0 \frac{\partial T}{\partial x_0} + v_0 \frac{\partial T}{\partial y_0} = \frac{1}{\rho} \frac{\partial}{\partial y_0} \left( \frac{\mu}{Pr} \frac{\partial T}{\partial y_0} \right) + m^* w_{\sim} (T_f - T_{\sim})$$

$$d) \quad \frac{\partial K_i}{\partial t} + u_0 \frac{\partial K_i}{\partial x_0} + v_0 \frac{\partial K_i}{\partial y_0} = \frac{1}{\rho} \frac{\partial}{\partial y_0} \left( \frac{\mu}{Sc} \frac{\partial K_i}{\partial y_0} \right) - w_{\sim} \quad (48)$$

where: 
$$w_{\sim} = \begin{cases} w_{\sim} & i \leq m^* \\ 0 & i = d \text{ (inert diluent gas)} \end{cases}$$

$$e) \quad K_p = 1 - K_d - \sum_{j=1}^{m^*} K_j$$

$$f) \quad w_{\sim} = b \left( \frac{p}{RT} \right)^{m^*-1} \exp[-E/RT] \prod_{j=1}^{m^*} K_j$$

$$g) \quad \rho = \frac{pM}{RT}$$

F. Transformation of Equations to the Corresponding Constant Density Plane

1. The Howarth Transformation

The set of relations presented in equation 48 is greatly simplified from the original relations of Sections II A and II B. The elimination of the density as an explicit dependent variable, however, would certainly lead to yet more tractable equations. Through the use of the so-called Howarth<sup>(55)</sup> or Dorodnitsyn<sup>(56)</sup> transformation, the lateral coordinate may be stretched in such a way as to effectively eliminate the density as an explicit dependent variable; the set of equations is thus effectively reduced to the constant density form. The Howarth transformation may thus be considered as a transformation from the real physical plane  $(x_0, y_0)$  in which the density is a variable, to a corresponding constant density plane  $(x, y)$ . The following transformation of independent variables is made:

$$\begin{aligned} x &= x_0 \\ y &= \int_0^{y_0} (\rho/\rho_x) dy_0 \end{aligned} \tag{49}$$

where  $\rho_x$  is the density of the combustible free stream. This variable transformation satisfies the differential relations:

$$\begin{aligned} \frac{\partial}{\partial x_0} \Big|_{y_0} &= \frac{\partial}{\partial x} \Big|_y + \frac{\partial y}{\partial x_0} \frac{\partial}{\partial y} \Big|_x \\ \frac{\partial}{\partial y_0} \Big|_{x_0} &= \frac{\rho}{\rho_x} \frac{\partial}{\partial y} \Big|_x \end{aligned} \tag{50}$$

where, from equation 49,

$$\frac{\partial y}{\partial x_0} = \int_0^y \frac{\partial}{\partial x_0} \left( \frac{\rho}{\rho_1} \right) dy_0 \quad (51)$$

The usual aerodynamic stream function,  $\Psi(x_0, y_0)$ , defined such that

$$\rho u_0 = \rho_1 \frac{\partial \Psi}{\partial y_0} \quad (52)$$

$$\rho v_0 = -\rho_1 \frac{\partial \Psi}{\partial x_0}$$

is now introduced. Combination of equations 50 and 52 yields the relations:

$$\rho u = \rho \frac{\partial \Psi}{\partial y} \quad (53)$$

$$\rho v = -\rho_1 \left[ \frac{\partial \Psi}{\partial x} + \frac{\partial \Psi}{\partial y} \frac{\partial y}{\partial x_0} \right]$$

The velocities in the transformed plane are now denoted by  $u$  and  $v$ , with:

$$u = \frac{\partial \Psi}{\partial y} \quad (54)$$

$$v = -\frac{\partial \Psi}{\partial x}$$

The following expressions are then obtained upon substituting equations 51 and 54 into equation 53:

$$\begin{aligned}
 u_0 &= u \\
 v_0 &= -\left(\rho_x/\rho\right)\left[-v + u\int_0^{y_0}\frac{\partial}{\partial x_0}\left(\rho/\rho_x\right)dy_0\right]
 \end{aligned}
 \tag{55}$$

Utilization of equations 19, 50, and 55 yields the following differential expressions:

$$u_0\frac{\partial}{\partial x_0} + v_0\frac{\partial}{\partial y_0} = u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y}
 \tag{56}$$

$$\frac{\partial}{\partial y_0}\left(\mu\frac{\partial}{\partial y_0}\right) = \frac{\rho}{\rho_x}\frac{\partial}{\partial y}\left(\frac{\mu\rho}{\rho_x}\frac{\partial}{\partial y}\right) = \rho v\frac{\partial^2}{\partial y^2}$$

where, by equation 19,  $\frac{\mu\rho}{\rho_x} = \frac{\mu_x\rho_x}{\rho_x} = \mu_x$ , and  $v \equiv \mu_x/\rho_x$  is the kinematic viscosity of the combustible free stream. Note that, as stated in Section IIC, the fortunate property that  $\mu\rho = \text{constant}$  for a gas mixture composed of mechanically similar Maxwellian molecules is essential to the fruitful application of the Howarth transformation.

If non-steady phenomena are eliminated from further consideration, the Howarth transformation of the relations in the physical plane, equation 48, according to equations 55 and 56 yields the following set of steady-state relations in the corresponding constant density plane:

Boundary layer type flow systems, corresponding constant density plane:

$$a) \quad \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

$$b) \quad u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = \nu \frac{\partial^2 u}{\partial y^2}$$

$$c) \quad u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \frac{\nu}{Pr} \frac{\partial^2 T}{\partial y^2} + m^* w_{\sim} (T_f - T_{\infty})$$

$$d) \quad u \frac{\partial K_i}{\partial x} + v \frac{\partial K_i}{\partial y} = \frac{\nu}{Sc} \frac{\partial^2 K_i}{\partial y^2} - w_i \quad ; i \neq p$$

where: 
$$w_i = \begin{cases} w_{\sim} & i \leq m^* \\ 0 & i = d \text{ (inert diluent gas)} \end{cases}$$

$$e) \quad K_p = 1 - K_d - \sum_{j=1}^{m^*} K_j$$

$$f) \quad w_{\sim} = b \left( \frac{p}{RT} \right)^{m^*-1} \exp(-E/RT) \prod_{j=1}^{m^*} K_j$$

$$g) \quad \rho = \frac{pM}{RT}$$

(57)

In the preceding equations, the results of Section IIC with regard to constant Prandtl and Schmidt numbers have been utilized.

The great simplification introduced by the Howarth transformation is now apparent. Note that the equations for the conservation of



mass and of momentum are now completely uncoupled from the equations of energy balance and of species continuity and are, in fact, reduced to the identical form of the constant density case. The solution of the velocity field in the plane of the transformation is thus reduced to a consideration of a pure mixing problem in the case of combustion in the laminar mixing region, or to a consideration of the incompressible laminar boundary layer on a flat plate in the case of combustion within the laminar boundary layer. These two problems have been solved and are discussed in the literature; Lock<sup>(57)</sup> and Görtler<sup>(58)</sup>, also reported by Pai<sup>(59)</sup>, have discussed the pure mixing problem and Blasius<sup>(60)</sup> has given the solution to the flat plate problem, which is also discussed in considerable detail by Schlichting<sup>(61)</sup>. The Howarth transformation has thus eliminated the added complication of combustion as far as the conservation equations for mass and momentum are concerned, and has simplified the remaining equations of energy balance and specie continuity.

## 2. Introduction of Dimensionless Dependent Variables

As a further step in preparing the governing equations for analysis, it will be convenient to express the dependent variables in dimensionless form. Before defining the dimensionless variables, however, it will be necessary to set apart one particular, and simple, special case: that of a laminar mixing region in which the two streams have the identical velocity prior to mixing. In this simple case no shear flow exists in the corresponding constant density plane ( $x, y$ ) and

the velocity is constant throughout the flow field in this plane\*. Thus for this particular case  $u = u_I$  and  $v = 0$  in equation 57, with the following result:

Shear-free mixing region †,  $u_I = u_{II}$ :

$$a) \quad \frac{\partial T}{\partial x} = \frac{v}{P u_x} \frac{\partial^2 T}{\partial y^2} + m^* \frac{w_{\sim}}{u_x} (T_f - T_x)$$

$$b) \quad \frac{\partial K_{\sim}}{\partial x} = \frac{v}{S_c u_x} \frac{\partial^2 K_{\sim}}{\partial y^2} - \frac{w_{\sim}}{u_x} \quad ; \quad \sim \neq p$$

$$\text{where:} \quad w_{\sim} = \begin{cases} w_{\sim} & \sim \leq m^* \\ 0 & \sim = d \end{cases}$$

(58)

$$c) \quad K_p = 1 - K_d - \sum_{j=1}^{m^*} K_j$$

$$d) \quad w_{\sim} = b \left( \frac{p}{RT} \right)^{m^*-1} \exp(-E/RT) \prod_{j=1}^{m^*} K_j$$

$$e) \quad \rho = \frac{pM}{RT}$$

\* When two streams having the same velocity but different temperatures mix in a constant pressure field, the resultant temperature gradient induces a shear-flow in the real, or physical plane  $(x_o, y_o)$ . Fortunately, however, the Howarth transformation warps this shear-flow in the  $x_o, y_o$  plane into an equivalent shear-free flow in the  $x, y$  plane of the transformation; in this latter plane, the streamlines are the lines  $y = \text{constant}$ .

† Hereafter, "shear-free flow" and "shear-flow" will refer to the flow conditions in the Howarth  $(x, y)$  plane, not to the conditions in the physical  $(x_o, y_o)$  plane.

The above particular case has been set apart at this time because certain of the dimensionless variables which are to be introduced in the general shear-flow case are infinite when  $u_I$  is equal to  $u_{II}$ .

Dimensionless streamwise velocity and temperature variables are now defined such that they are equal to unity at the cold boundary (denoted by the subscript I) and vanish at the hot boundary (denoted by the subscript II). A new dimensionless concentration variable is also defined which will later prove to be of a useful form. The following dimensionless variables and parameters are now introduced:

$$\left. \begin{aligned}
 U(x,y) &= \frac{u(x,y) - u_{II}}{u_I - u_{II}} \\
 V(x,y) &= \frac{v(x,y) - u_{II}}{u_I - u_{II}} \\
 Z(x,y) &= \frac{T_{II} - T(x,y)}{T_{II} - T_I} \\
 G_i(x,y) &= C_i [K_i(x,y) - K_{i,II}] \\
 &\quad i \neq p
 \end{aligned} \right\} \begin{aligned}
 u_I &\neq u_{II} \\
 \beta_1 &= E/\alpha T_{II} \\
 C_1 &= m^* \left( \frac{T_{II} - T_I}{T_{II} - T_I} \right) \\
 C_2 &= \frac{T_{II} - T_I}{2T_{II}}
 \end{aligned} \quad (59)$$

It should be noted that in the definition of the dimensionless expressions above, it has been implicitly assumed that the physical quantities are constant along both the hot and the cold boundaries. This assumption is essential to the manner in which the above expressions are to be utilized in obtaining equation 61 and following relations. Thus, in the case of combustion within the laminar boundary layer on a flat plate for example, the wall temperature must be a constant and arbitrary wall

temperature distributions are a priori ruled out when the above dimensionless quantities are employed in the manner which follows. In all analyses in the main body of the text, therefore, the physical quantities will be constant along both the hot and the cold boundaries. These boundaries, of course, have yet to be specified. The case of the laminar boundary layer on a flat plate with arbitrary wall temperature distribution is treated in Appendix F by a different technique.

The reaction term, equation 27, will be considerably simplified if the dimensional parameter  $C_3(\text{cm}^{-1})$  and the dimensionless variable  $\Theta_{\sim}(x, y)$  are also introduced:

$$C_3 = \begin{cases} \left( \frac{b}{u_I - u_{II}} \right) \left( \frac{\rho}{R T_{II}} \right)^{m^* - 1} & ; u_I \neq u_{II} \\ \left( \frac{b}{u_I} \right) \left( \frac{\rho}{R T_{II}} \right)^{m^* - 1} & ; u_I = u_{II} \end{cases} \quad (60)$$

$$\Theta_{\sim}(x, y) = \left[ 1 - 2c_2 z(x, y) \right]^{1 - m^*} \prod_{j=1}^{m^*} K_j \cdot \exp \left[ \frac{-\beta_1}{1 - 2c_2 z(x, y)} \right]$$

Through the use of equations 59 and 60, the set of relations for the general shear-flow case,  $u_I \neq u_{II}$ , given by equation 57, can be simplified to the following form:

Shear-flow,  $u_I \neq u_{II}$ :

$$a) \quad \frac{\partial \sigma}{\partial x} + \frac{\partial \tau}{\partial y} = 0$$

$$b) \quad \left( \sigma + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial \sigma}{\partial x} + \left( \tau + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial \tau}{\partial y} = \frac{1}{\sigma} \frac{\partial^2 \sigma}{\partial y^2}$$

$$c) \quad \left( \sigma + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial \tau}{\partial x} + \left( \tau + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial \tau}{\partial y} = \frac{1}{\sigma \rho} \frac{\partial^2 \tau}{\partial y^2} - c_1 c_3 \theta_{\sim}(x, y)$$

$$d) \quad \left( \sigma + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial G_i}{\partial x} + \left( \tau + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial G_i}{\partial y} = \frac{1}{\sigma s_c} \frac{\partial^2 G_i}{\partial y^2} - c_1 c_3 \theta_{\sim}(x, y)$$

$i \neq p$

where:

$$\theta_{\sim}(x, y) = \begin{cases} \theta_{\sim}(x, y) & i \leq m^* \\ 0 & i = d \end{cases}$$

(61)

$$e) \quad K_{\sim} = K_{\sim II} + \frac{G_{\sim}}{c_i} \quad ; \quad i \neq p$$

$$f) \quad K_p = 1 - K_d - \sum_{j=1}^{m^*} K_j$$

$$g) \quad S = \frac{pM}{RT} \quad ; \quad T = T_{II} - (T_{II} - T_I) z$$

$$h) \quad \Lambda = u_{II}/u_I$$

Although the above equations can be considerably simplified in the case of the laminar boundary layer on a flat plate, since in this case  $\Lambda = u_{II}/u_I = 0$ , the general form presented will be maintained in order to permit application to the laminar mixing region, where  $\Lambda$  may be non-zero.

Through the use of equations 59 and 60, the set of governing relations for the special shear-free case,  $u_I = u_{II}$ , given by equation 58 can be simplified to the following form:

Shear-free flow,  $u_I = u_{II}$ :

$$a) \quad \frac{\partial \eta}{\partial x} = \frac{1}{\sigma Pr} \frac{\partial^2 \eta}{\partial y^2} - c_1 c_3 \theta_{\sim}(x, y)$$

$$b) \quad \frac{\partial G_{\lambda}}{\partial x} = \frac{1}{\sigma Sc} \frac{\partial^2 G_{\lambda}}{\partial y^2} - c_1 c_3 \theta_{\lambda}(x, y) \quad ; \lambda \neq p$$

$$\text{where: } \theta_{\lambda} = \begin{cases} \theta_{\sim} & \lambda \leq m^* \\ 0 & \lambda = d \end{cases}$$

$$c) \quad K_{\lambda} = K_{\lambda II} + \frac{G_{\lambda}}{c_1} \quad ; \lambda \neq p$$

$$d) \quad K_p = 1 - K_d - \sum_{j=1}^{m^*} K_j$$

$$e) \quad \rho = \frac{\rho M}{RT} \quad ; \quad T = T_{II} - (T_{II} - T_I) \eta$$

(62)

In the above equations, the quantity

$$\sigma = \begin{cases} u_I/v = u_I \rho_I/\mu_I & ; u_I = u_{II} \\ (u_I - u_{II})/v = (u_I - u_{II}) \rho_I/\mu_I & ; u_I \neq u_{II} \end{cases} \quad (63)$$

has the dimensions of Reynolds number per unit length ( $\text{cm}^{-1}$ ) based on the gas properties of the cold combustible free stream.

### G. Similarity Solutions for the Specie Concentrations

#### 1. Similarity of Specie Continuity and Energy Balance

##### Equations When $Pr = Sc$ :

The governing relations presented in equations 61 and 62 for boundary layer type flow systems with one-step chemical reactions are the end result of rather considerable and somewhat drastic simplifications. They are, however, still non-linear and are so complex that an exact analytic solution is not to be expected. Useful approximate analytic solutions, however, may be obtained for various special cases. In particular, the special case where the Prandtl and Schmidt numbers are equal is amenable to a relatively simple analysis which may readily be applied to first-order, second-order, and third-order chemical reactions occurring either in the laminar mixing region or in the laminar boundary layer on a flat plate.

In view of the rather drastic assumptions which have already been made and the power of this simple assumption, the restriction to the particular case where the Prandtl and Schmidt numbers are equal will not unduly limit the usefulness of the present analysis which, as frequently stated, is exploratory rather than quantitative in nature.

Throughout the remainder of the present paper, then, the assumption of equal Prandtl and Schmidt numbers will consistently be made:

$$\text{Pr} = \text{Sc} \quad (64)$$

From equations 18 and 64 it is apparent that  $\rho D_c \nu / \lambda = 1$ . This relation infers that the rate of energy transfer by thermal conduction is exactly equal to the rate of energy transfer by diffusion\*. This approximation is in fair accord with reality in many combustion problems.

By virtue of equation 64, a striking similarity now exists between the reactant specie ( $i \leq m^*$ ) continuity relations and the energy balance relation in equations 61 and 62; the mathematical form, though not necessarily the boundary conditions, are now identical. Now if each of the reactant specie continuity relations in equations 61 and 62 are subtracted from the corresponding energy balance relation, then equation 61d may be replaced by the following expressions,

$$\left. \begin{aligned} \left( \nabla + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial}{\partial x} (z - G_i) + \left( \nabla + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial}{\partial y} (z - G_i) &= \frac{1}{\sigma_{Pr}} \frac{\partial^2}{\partial y^2} (z - G_i) \\ & \quad i \leq m^* \\ \left( \nabla + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial G_i}{\partial x} + \left( \nabla + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial G_i}{\partial y} &= \frac{1}{\sigma_{Pr}} \frac{\partial^2 G_i}{\partial y^2} \quad ; i = d \end{aligned} \right\} (65)$$

and similarly, equation 62b may be replaced by the expressions:

$$\left. \begin{aligned} \frac{\partial}{\partial x} (z - G_i) &= \frac{1}{\sigma_{Pr}} \frac{\partial^2}{\partial y^2} (z - G_i) \quad ; i \leq m^* \\ \frac{\partial G_i}{\partial x} &= \frac{1}{\sigma_{Pr}} \frac{\partial^2 G_i}{\partial y^2} \quad ; i = d \end{aligned} \right\} (66)$$

---

\* Another physical statement corresponding to equation 64 is that the ratio of macroscopic transport to microscopic transport is the same for both heat and mass transport.



The boundary conditions for each of the above expressions are normally different. By utilization of a properly chosen dimensionless variable, however, each of the above sets of  $m^* + 1$  partial differential equations can be reduced to a single partial differential equation having normalized boundary conditions of zero and unity. The dimensionless variable utilized, which has the same boundary conditions as  $\bar{U}(x, y)$  and  $\bar{Z}(x, y)$ , is defined as follows:

$$\begin{aligned}
 \text{a) } F(x, y) &\equiv \left[ \begin{aligned} &\left[ \frac{\bar{Z}(x, y) - G_{i, \text{I}}(x, y)}{\bar{Z}_{\text{I}} - G_{i, \text{I}}} \right] = \left[ \frac{\bar{Z} - c_i (K_i - K_{i, \text{I}})}{1 - c_i \Delta_i} \right] && ; i \leq m^* \\ &\frac{G_{i, \text{I}}(x, y)}{G_{i, \text{I}}} = \frac{K_i - K_{i, \text{I}}}{\Delta_i} && ; i = d \end{aligned} \right] \quad (67)
 \end{aligned}$$

where:

$$\text{b) } \Delta_i = K_{i, \text{I}} - K_i$$

The following expressions for the reactant and inert diluent specie weight fractions in terms of the dimensionless variable  $F(x, y)$  are obtained from equation 67. The expression for the product specie weight fraction is obtained by substituting the expressions for the reactant and inert species into equation 61 f (or equation 62 d) and simplifying; it is assumed that the product specie weight fraction is zero at the cold boundary.

$$\begin{aligned}
 \text{a)} \quad K_{\lambda} &= K_{\lambda_{II}} + \Delta_{\lambda} F + \frac{1}{c_1} (\beta - F) \quad ; \lambda \leq m^* \\
 \text{b)} \quad K_d &= K_{d_{II}} + \Delta_d F \\
 \text{c)} \quad K_p &= K_{p_{II}} (1-F) - \frac{m^*}{c_1} (\beta - F)
 \end{aligned} \tag{68}$$

The following set of governing relations for shear-flow,  $u_I \neq u_{II}$ , with  $Pr = Sc$  is obtained upon substituting equation 67a into equation 65, using the resultant expression to replace equation 61d, and replacing equations 61e and 61f by equation 68.

Shear-flow,  $u_I \neq u_{II}$ , with  $Pr = Sc$ :

$$\begin{aligned}
 \text{a)} \quad \frac{\partial \sigma}{\partial x} + \frac{\partial \tau}{\partial y} &= 0 \\
 \text{b)} \quad \left( \sigma + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial \sigma}{\partial x} + \left( \tau + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial \tau}{\partial y} &= \frac{1}{\sigma} \frac{\partial^2 \sigma}{\partial y^2} \\
 \text{c)} \quad \left( \sigma + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial \beta}{\partial x} + \left( \tau + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial \beta}{\partial y} &= \frac{1}{\sigma Pr} \frac{\partial^2 \beta}{\partial y^2} - c_1 c_3 \theta_{\lambda}(x, y) \\
 \text{d)} \quad \left( \sigma + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial F}{\partial x} + \left( \tau + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial F}{\partial y} &= \frac{1}{\sigma Pr} \frac{\partial^2 F}{\partial y^2} \\
 \text{e)} \quad K_{\lambda} &= K_{\lambda_{II}} + \Delta_{\lambda} F + \frac{1}{c_1} (\beta - F) \quad ; \lambda \leq m^* \\
 \text{f)} \quad K_d &= K_{d_{II}} + \Delta_d F \\
 \text{g)} \quad K_p &= K_{p_{II}} (1-F) - \frac{m^*}{c_1} (\beta - F) \\
 \text{h)} \quad \beta &= \frac{PM}{RT} \quad ; \quad T = T_{II} - (T_{II} - T_I) \beta
 \end{aligned} \tag{69}$$

The following set of governing relations for shear-free flow,  $u_I = u_{II}$ , with  $Pr = Sc$  is obtained upon substituting equation 67a into equation 66, using the resultant expression to replace equation 62b, and replacing equations 62c and 62d by equation 68.

Shear-free flow,  $u_I = u_{II}$ , with  $Pr = Sc$ :

$$\begin{aligned}
 \text{a) } \quad \frac{\partial z}{\partial x} &= \frac{1}{\sigma Pr} \frac{\partial^2 z}{\partial y^2} - c_1 c_3 \theta_{\infty}(x, y) \\
 \text{b) } \quad \frac{\partial F}{\partial x} &= \frac{1}{\sigma Pr} \frac{\partial^2 F}{\partial y^2} \\
 \text{c) } \quad K_{\lambda} &= K_{\lambda II} + \Delta_{\lambda} F + \frac{1}{c_1} (z - F) \quad ; \lambda \leq m^* \\
 \text{d) } \quad K_d &= K_{d II} + \Delta_d F \\
 \text{e) } \quad K_p &= K_{p II} (1 - F) - \frac{m^*}{c_1} (z - F) \\
 \text{f) } \quad \rho &= \frac{\rho M}{\rho T} \quad ; \quad T = T_{II} - z(T_{II} - T_I)
 \end{aligned}
 \tag{70}$$

The boundary conditions on the partial differential relations in equations 69 and 70 are particularly simple by virtue of the definitions of the dimensionless variables which have been introduced:

Conditions at the cold boundary:

$$\vartheta(x, y) = z(x, y) = F(x, y) = 1$$

Conditions at the hot boundary:

$$\vartheta(x, y) = z(x, y) = F(x, y) = 0$$

(71)

2. Similarity of the  $F(x, y)$  function equation with the momentum equation when  $Pr = 1$ :

One additional and particularly powerful similarity can be found in the shear-flow case. If the Prandtl number is set equal to unity, it is apparent from the resulting complete similarity of equations 69b and 69d and the identical boundary conditions, equation 71, that the function  $F(x, y)$  must be equivalent to the dimensionless velocity  $\bar{U}(x, y)$ . Thus,

$$F(x, y) = \bar{U}(x, y) \tag{72}$$

when:  $Pr = 1$

This similarity between the  $F(x, y)$  function equation and the momentum equation reduces the set of governing equations which remain to be solved to the relations for the conservation of mass and momentum and the energy balance equation.

The following set of governing equations for the particular case where  $Pr = Sc = 1$  is obtained upon substituting equation 72 into equations 69e, 69f, and 69g and deleting equation 69d by virtue of equation 72.

Shear-flow,  $u_I \neq u_{II}$ , with  $Pr = Sc = 1$ :

$$\begin{aligned}
 \text{a)} \quad & \frac{\partial \sigma}{\partial x} + \frac{\partial \sigma}{\partial y} = 0 \\
 \text{b)} \quad & \left( \sigma + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial \sigma}{\partial x} + \left( \sigma + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial \sigma}{\partial y} = \frac{1}{\sigma} \frac{\partial^2 \sigma}{\partial y^2} \\
 \text{c)} \quad & \left( \sigma + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial \theta}{\partial x} + \left( \sigma + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial \theta}{\partial y} = \frac{1}{\sigma} \frac{\partial^2 \theta}{\partial y^2} - c_1 c_3 \theta_n(x, y) \\
 \text{d)} \quad & K_i = K_{i_{II}} + \Delta_i \sigma + \frac{1}{c_i} (z - \sigma) \quad ; \quad i \leq m^* \\
 \text{e)} \quad & K_d = K_{d_{II}} + \Delta_d \sigma \\
 \text{f)} \quad & K_p = K_{p_{II}} (1 - \sigma) - \frac{m^*}{c_i} (z - \sigma) \\
 \text{g)} \quad & \rho = \frac{\rho M}{R T} \quad ; \quad T = T_{II} - (T_{II} - T_I) z
 \end{aligned} \tag{73}$$

For the preceding particular case,  $Pr = Sc = 1$ , it follows from equation 18 that the assumption is implicitly being made that the rates of heat transfer by convection, by conduction, and by diffusion are all equal. Obviously, therefore, the solution of equation 73 will not yield information directly related to the differences in the heat transfer rates by the three mechanisms listed above. The solution of equation 73 will, however, provide considerable insight into the qualitative aspects of combustion in shear-flow regions.

It should be noted that a powerful similarity relation similar to that presented in paragraph 1 above is equally applicable to the one-dimensional flow case, equation 47, when  $Pr = Sc$ . Similarity solutions for the one-dimensional case are briefly discussed in Appendix E.

#### H. The Blasius Transformation

Since the governing relations in equations 69, 70, and 73 are in the same mathematical form as the usual incompressible equations, the introduction of the Blasius type variables  $\eta$  and  $s$  in place of the present variables  $y$  and  $x$  will be of considerable benefit. Define

$$\eta = \frac{y}{2} \sqrt{\frac{W}{\nu x}} \quad (74)$$

where the quantity  $W$  has the dimensions of velocity and is given by,

$$W = \begin{cases} u_I; & \text{if } u_I = u_{II} \text{ or if } u_I > 0 \\ & \text{and } u_{II} = 0 . \\ \\ u_I - u_{II}; & \text{if } u_I \neq u_{II} \\ & \text{and } u_{II} \neq 0 \end{cases} \quad (75)$$

Then for a change of variables  $x, y$  to  $s, \eta$ , the following differential relations will apply:

$$\begin{aligned} \frac{\partial}{\partial x} \Big|_y &= \frac{\partial s}{\partial x} \Big|_y \frac{\partial}{\partial s} \Big|_\eta + \frac{\partial \eta}{\partial x} \Big|_y \frac{\partial}{\partial \eta} \Big|_s \\ \frac{\partial}{\partial y} \Big|_x &= \frac{\partial s}{\partial y} \Big|_x \frac{\partial}{\partial s} \Big|_\eta + \frac{\partial \eta}{\partial y} \Big|_x \frac{\partial}{\partial \eta} \Big|_s \end{aligned}$$

If now  $s = x$  and equation 74 is utilized, then

$$\begin{aligned}
 (a) \quad \frac{\partial}{\partial x} \Big|_y &= \frac{\partial}{\partial x} \Big|_\eta - \frac{\eta}{2x} \frac{\partial}{\partial \eta} \Big|_x \\
 (b) \quad \frac{\partial}{\partial y} \Big|_x &= \frac{1}{2} \left( \frac{W}{vX} \right)^{1/2} \frac{\partial}{\partial \eta} \Big|_x \\
 (c) \quad \frac{\partial^2}{\partial y^2} \Big|_x &= \frac{1}{4} \left( \frac{W}{vX} \right) \frac{\partial^2}{\partial \eta^2} \Big|_x
 \end{aligned} \tag{76}$$

Upon substituting the above differential relations into equation 70, the following set of governing equations in the  $\eta, x$  plane is obtained for the shear-free,  $u_I = u_{II}$ , case.

Shear-free flow,  $u_I = u_{II}$ , with  $Pr = Sc$ :

$$\begin{aligned}
 (a) \quad \frac{\partial^2 \theta}{\partial \eta^2} + 2Pr \eta \frac{\partial \theta}{\partial \eta} &= 4Pr x \frac{\partial \theta}{\partial x} + 4Pr x c_1 c_3 \theta_2(\eta, x) \\
 (b) \quad \frac{\partial^2 F}{\partial \eta^2} + 2Pr \eta \frac{\partial F}{\partial \eta} &= 4Pr x \frac{\partial F}{\partial x} \\
 (c) \quad K_i &= K_{i, II} + \frac{1}{c_i} (z - F) + \Delta_i F \quad ; i \leq m^* \\
 (d) \quad K_d &= K_{d, II} + \Delta_d F \\
 (e) \quad K_p &= K_{p, II} (1 - F) - \frac{m^*}{c_i} (z - F) \\
 (f) \quad \rho &= \frac{\rho M}{\rho T} \quad ; \quad T = T_{II} - (T_{II} - T_I) z
 \end{aligned} \tag{77}$$

In the general shear-flow case, the dependent variable  $f(\eta)$  is now defined such that,

$$\Psi(\eta, x) = (wvx)^{1/2} f(\eta) \quad (78)$$

where  $\Psi(\eta, x)$  is the usual aerodynamic stream function expressed in terms of the  $\eta$ ,  $x$  coordinates. It follows from equations 54, 59, 75, 76, and 78 that,

$$(a) \quad \left( U + \frac{\Lambda}{1-\Lambda} \right) = \frac{1}{2} f'(\eta) \quad (79)$$

$$(b) \quad \left( V + \frac{\Lambda}{1-\Lambda} \right) = \frac{1}{2} \left( \frac{v}{wx} \right)^{1/2} \left[ \eta f'(\eta) - f(\eta) \right]$$

where the prime denotes a differentiation with respect to  $\eta$ . Thus, from equations 76 and 79,

$$\left( U + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial}{\partial x} \Big|_y + \left( V + \frac{\Lambda}{1-\Lambda} \right) \frac{\partial}{\partial y} \Big|_x = \frac{1}{2} \left[ f'(\eta) \frac{\partial}{\partial x} \Big|_\eta - \frac{f(\eta)}{2x} \frac{\partial}{\partial \eta} \Big|_x \right] \quad (80)$$

Differentiation of equation 79a yields:

$$\frac{\partial U}{\partial x} \Big|_\eta = 0 ; \quad \frac{\partial U}{\partial \eta} \Big|_x = \frac{1}{2} f''(\eta) ; \quad \frac{\partial^2 U}{\partial \eta^2} \Big|_x = \frac{1}{2} f'''(\eta) \quad (81)$$

Upon substituting equations 76, 80, and 81 into equation 70 the following set of governing equations in the  $\eta$ ,  $x$  plane is obtained for the shear-flow case,  $u_I \neq u_{II}$ , with  $Pr = Sc \neq 1$ :



Shear-flow,  $u_I \neq u_{II}$ , with  $Pr = Sc$ :

$$(a) \quad f'''(\eta) + f(\eta)f''(\eta) = 0$$

$$(b) \quad \frac{\partial^2 z}{\partial \eta^2} + Pr f(\eta) \frac{\partial z}{\partial \eta} = 2 Pr X f'(\eta) \frac{\partial z}{\partial X} + 4 Pr X C_1 C_3 \Theta_{\infty}(\eta, X)$$

$$(c) \quad \frac{\partial^2 F}{\partial \eta^2} + Pr f(\eta) \frac{\partial F}{\partial \eta} = 2 Pr X f'(\eta) \frac{\partial F}{\partial X}$$

$$(d) \quad K_i = K_{i,II} + \frac{1}{c_i} (z - F) + \Delta_i F \quad ; \quad i \leq m^* \quad (82)$$

$$(e) \quad K_d = K_{d,II} + \Delta_d F$$

$$(f) \quad K_p = K_{p,II} (1 - F) - \frac{m^*}{c_i} (z - F)$$

$$(g) \quad U = \frac{u - u_{II}}{u_I - u_{II}} = \frac{1}{2} f'(\eta) - \frac{\Lambda}{1 - \Lambda}$$

$$(h) \quad \theta = \frac{PM}{QT} \quad ; \quad T = T_{II} - (T_{II} - T_I) z$$

The following set of equations for the shear-flow case,  $u_I \neq u_{II}$ , with  $Pr = Sc = 1$ , is obtained upon simplifying equation 73 according to equations 76, 79, 80, and 81.

Shear-flow,  $u_I \neq u_{II}$ , with  $Pr = Sc = 1$ :

$$(a) \quad f'''(\eta) + f(\eta)f''(\eta) = 0$$

$$(b) \quad \frac{\partial^2 z}{\partial \eta^2} + f(\eta) \frac{\partial z}{\partial \eta} = 2xf'(\eta) \frac{\partial z}{\partial x} + 4xC_1C_3\theta_{\sim}(\eta, x)$$

$$(c) \quad K_i = K_{i_{II}} + \frac{1}{C_i}(z - \sigma) + \Delta_i \sigma \quad ; \quad i \leq m^*$$

$$(d) \quad K_d = K_{d_{II}} + \Delta_d \sigma$$

$$(e) \quad K_p = K_{p_{II}}(1 - \sigma) - \frac{m^*}{C_1}(z - \sigma)$$

$$(f) \quad \sigma = \frac{u - u_{II}}{u_I - u_{II}} = \frac{1}{2}f'(\eta) - \frac{\Lambda}{1 - \Lambda}$$

$$(g) \quad S = \frac{PM}{QT} \quad ; \quad T = T_{II} - (T_{II} - T_I)z$$

(83)

In the above,  $\Lambda = u_{II}/u_I$  is the velocity ratio of the two streams prior to mixing in the mixing region case and is equal to zero in the boundary layer case.

The boundary conditions corresponding to equations 77, 82, and 83 are obtained from equations 72 and 79.

Conditions at the cold boundary:

$$\begin{aligned} g(\eta, x) &= F(\eta, x) = 1 \\ f'(\eta) &= \frac{2}{1-\Lambda} \quad ; \quad \Lambda \neq 1 \end{aligned}$$

Conditions at the hot boundary:

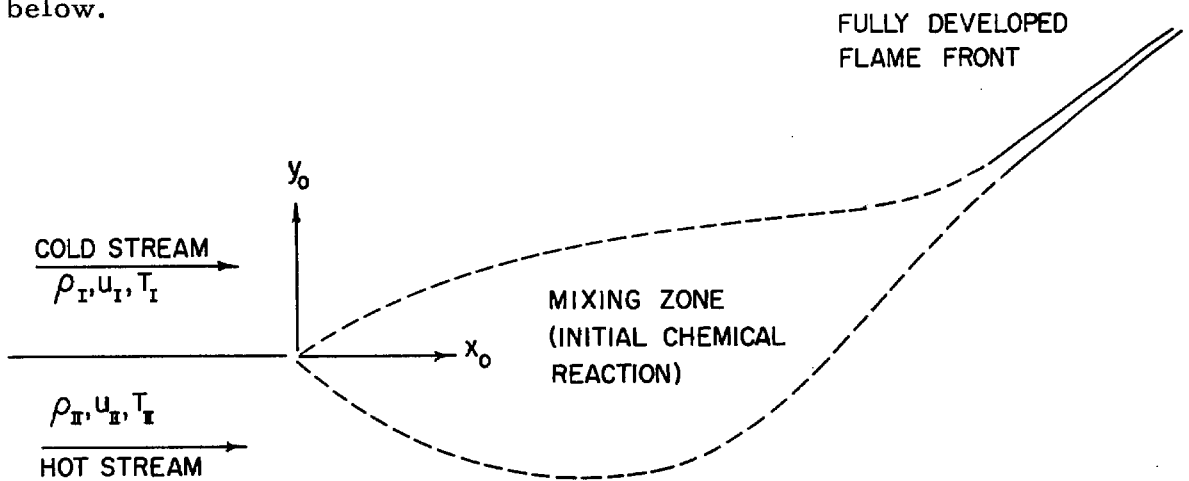
$$\begin{aligned} g(\eta, x) &= F(\eta, x) = 0 \\ f'(\eta) &= \frac{2\Lambda}{1-\Lambda} \quad ; \quad \Lambda \neq 1 \end{aligned}$$

(84)

### III. COMBUSTION IN THE SHEAR-FREE LAMINAR MIXING REGION, STREAM VELOCITIES EQUAL, WITH $Pr = Sc$ :

#### A. Formulation of the Combustion Problem in the Laminar Mixing Region

Consider two semi-infinite steady gas streams flowing from left to right parallel to the  $x_0$  axis in the physical plane. The upper stream consists of a cold gas mixture at temperature  $T_I$ , density  $\rho_I$ , and velocity  $u_I$ . The lower stream consists of a hot gas mixture at temperature  $T_{II}$ , density  $\rho_{II}$ , and velocity  $u_{II}$ . The specification of the constituents of the two gas streams is dependent upon the order of chemical kinetics being considered and will thus be treated in Sections IIIC and IIID where first-order and second-order reactions respectively are considered. For the present, it is sufficient to state that the constituents are such that upon the mixing of the two streams (and only upon such mixing) an exothermic chemical reaction can take place. The model which serves as a basis for the analysis is presented below.



From the sketch and the definition of  $\eta$ , equation 74, it should be clear that the cold and hot boundaries are defined by  $\eta = +\infty$  and  $\eta = -\infty$  respectively in the  $\eta, x$  plane of the analysis. Throughout the mixing region the reaction rate increases until at some inclined front downstream of the point  $x_0 = 0$ , the reaction rate reaches its maximum value and a flame front is established as indicated in the sketch.

It will be assumed that the lower, hot stream is at a temperature which is less than the adiabatic flame temperature for the combustible mixture. The transport phenomena of heat transfer and diffusion of chemical specie must thus govern the ignition and initial reaction rate. As a consequence it follows that there will be a region immediately downstream of the initiation of mixing in which the effects of chemical reaction are small and in which the chemical concentration and temperature fields differ only slightly from those of a classic mixing problem without chemical reaction.

The velocity and temperature profiles found in the classic mixing problem are presented in figure 1, which is similar to a figure given by Lock<sup>(57)</sup>. The profiles prior to mixing are smoothed during the mixing process by viscosity in the case of velocity and by heat transfer, through the mechanisms of conduction, convection, and diffusion, in the case of temperature. The anticipated chemically induced changes in the temperature distribution when reaction takes place are presented in figure 2; this figure is taken from a paper by Marble and Adamson<sup>(8)</sup> which will be discussed in Section III B.

The initial profile prior to mixing is the same as for the classic mixing case without chemical reaction. Then, for a short distance downstream of the initiation of mixing, the heat addition due to chemical reaction is small, as indicated by the dotted line in the second profile. At a given value of  $y$  (or of  $\eta$ ), the heat addition due to chemical reaction continues to increase until at some point downstream the local temperature exceeds the lower, hot stream temperature and a temperature bulge is formed as shown by the solid line in the third profile. This temperature bulge grows rapidly in magnitude and moves upward (or downward, depending upon initial conditions) toward the region of higher combustible concentration. A laminar flame front is finally established as is indicated by the dotted line in the third profile. With the establishment of the flame front, the local temperature is essentially at the adiabatic flame temperature. Note that steep reaction induced temperature gradients are associated with the laminar flame front.

It was pointed out on page 40 that the application of the boundary layer assumptions, which are fundamental to the present analysis, is valid only when the reaction induced gradients in the temperature and in the other physical variables are substantially greater in the lateral direction than in the streamwise direction. Since steep temperature gradients exist normal to a laminar flame front, it follows that the flame must lie at a very small angle with respect to the  $x_0$  or flow axis if the boundary layer assumptions are to be valid throughout the entire mixing and flame region. This implies that if  $u_n$  is the flame speed (normally of the order of one to ten feet per second), then  $u_n/u_1$  and

$u_n/u_{II}$  must both be small compared to unity in order to validate the boundary layer assumptions throughout the mixing and flame region. Fortunately, even if the above inequalities do not hold, the boundary layer assumptions are valid throughout most of the mixing region of interest and break down only at the incipience of a fully developed flame front having steep temperature gradients. As was pointed out by Adamson<sup>(62)</sup>, the only result of increasing the initial flow velocities so that both of the above inequalities are valid is to allow computation of a flame speed and flame thickness, results which can be obtained by a much simpler one-dimensional analysis.

In conclusion, the mixing region analysis to be presented in the following three sections will be concerned only with the initial zone in which the reaction induced changes and the streamwise gradients in the physical variables are small; the boundary layer assumptions will thus be valid throughout the region of present interest regardless of flow velocities. Furthermore, as a consequence of the fact that the reaction induced variations are small in the region of interest, these variations may be treated as perturbations to the pure mixing region and an iterative solution for the mixing region with chemical reaction may be obtained.

B. General Solution for the Case of Equal Stream Velocities with  
 $Pr = Sc$ :

Marble and Adamson<sup>(8)</sup> have obtained an analytic first-approximation to the solution for the particular case of a first-order reaction occurring in a laminar mixing region. The classic perturbation tech-

nique is employed for the region of initial chemical reaction and the solution is then extended throughout the flame zone by an extension of the von Kármán integral method. They start with a set of relations which is equivalent, though not of identical form, with equation 57 and primarily consider the case where the stream velocities are equal prior to mixing (the shear-free case, equation 58). A method of extending their solution (by utilization of the asymptotic expansions of the solution for the velocity field) to any case in which the velocity ratio is not too small is, however, indicated<sup>(8)</sup>. No restrictions on the values of the Prandtl and Schmidt numbers other than that they be constant for the mixture are imposed. An extensive treatment of this interesting analysis is presented in reference 62.

Pai<sup>(10)</sup> has also studied the problem of a first-order reaction occurring in a laminar mixing region with equal stream velocities. His basic assumptions and approach are identical with those of the Marble-Adamson analysis. Except for his utilization of the stream function as an independent variable instead of the  $\eta$  or Blasius type independent variable employed by Marble and Adamson, his analysis for the region of initial chemical reaction is also identical\*.

The extension of the Marble-Adamson analysis (or of Pai's equivalent analysis) to the treatment of chemical reactions which follow second-order or third-order kinetics is not straightforward. Further-

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\* Pai employs the von Mises transformation; Marble and Adamson employ the Howarth transformation. The results of these two transformations are equivalent in the present application.



more, extension of their analysis to a higher-order solution (obtaining more terms in their perturbation series) is difficult. The present analysis, which draws heavily from the work of Marble and Adamson, requires the restriction of equal Prandtl and Schmidt numbers, but has the advantage of being easily applied to first-order, second-order, or to third-order reactions; furthermore, any desired mathematical-order of solution may be obtained by a straightforward iteration process, and all finite values of the velocity ratio may be considered.

In the present section a general solution which is valid for first-order, second-order, and third-order reactions occurring in the shear-free mixing region (velocity ratio equal to unity) is obtained. Detailed solutions for a first-order reaction are presented in Section III B. Detailed solutions for a second-order reaction, including the effects of changes in the fuel-air ratio and in the dilution of the combustible mixture by an inert gas, are presented in Section III C. The shear-flow mixing region (velocity ratio not equal to unity) is considered in Part IV.

The governing equations and corresponding boundary conditions for combustion in the laminar shear-free mixing region with  $Pr = Sc$  are directly obtainable from equations 77 and 84. By virtue of the similarity solution for  $Pr = Sc$  (Section II G. 1) only two equations remain to be solved. As noted in Section III A, the cold and hot boundaries for the mixing region are  $\eta = +\infty$  and  $\eta = -\infty$  respectively.

$$\begin{aligned}
 \text{a)} \quad & \frac{\partial^2 z}{\partial \eta^2} + 2Pr \eta \frac{\partial z}{\partial \eta} = 4Prx \frac{\partial z}{\partial x} + 4Prx C_1 C_3 \theta_n(\eta, x) \\
 & \text{with: } z(\eta, x) = \begin{cases} 1 & ; \eta = +\infty \\ 0 & ; \eta = -\infty \end{cases} \\
 \text{b)} \quad & \frac{\partial^2 F}{\partial \eta^2} + 2Pr \eta \frac{\partial F}{\partial \eta} = 4Prx \frac{\partial F}{\partial x} \\
 & \text{with: } F(\eta, x) = \begin{cases} 1 & ; \eta = +\infty \\ 0 & ; \eta = -\infty \end{cases}
 \end{aligned} \tag{85}$$

The other unknowns are obtained upon substituting the solutions to the preceding equations into the following expressions from equation 77.

$$\begin{aligned}
 \text{a)} \quad & K_i = K_{i\infty} + \frac{1}{c_i} (z - F) + \Delta_i F \quad ; \quad i \leq m^* \\
 \text{b)} \quad & K_d = K_{d\infty} + \Delta_d F \\
 \text{c)} \quad & K_p = K_{p\infty} (1 - F) - \frac{m^*}{c_i} (z - F) \\
 \text{d)} \quad & S = \frac{pM}{RT} \quad ; \quad T = T_{\infty} - (T_{\infty} - T_I) z
 \end{aligned} \tag{86}$$

The form of equation 85b and the corresponding boundary conditions indicate that  $F(\eta, x) \equiv F(\eta)$ , thus

$$\left. \begin{aligned} \frac{d^2 F}{d\eta^2} + 2Pr\eta \frac{dF}{d\eta} &= 0 \\ F(\eta) &= \begin{cases} 1 & \eta = +\infty \\ 0 & \eta = -\infty \end{cases} \end{aligned} \right\} \quad (87)$$

The solution of equation 87 is obtained in Appendix B-1; the result is,

$$\left. F(\eta) = \frac{1}{2} [1 + \operatorname{erf}(\eta\sqrt{Pr})] \right\} \quad (88)$$

where  $\operatorname{erf} x$  denotes the tabulated error function of  $x$ ; cf. Appendix B, page 161. The solution to equation 85a is not to be obtained so easily. However, as previously noted, this analysis is concerned with the initial region in which the reaction induced changes in the physical quantities, temperature included, are relatively small. A close approximation to the dimensionless temperature profile, namely that for the classic mixing problem without chemical reaction, can thus be obtained as a basis for an iterative solution. The dimensionless temperature for the classic mixing problem, which will be denoted by the symbol  $z^{(0)}(\eta, x)$ , is given by equation 85a with the reaction term, the last term, set equal to zero. Thus,

$$\left. \begin{aligned} \frac{\partial^2 z^{(0)}}{\partial \eta^2} + 2Pr\eta \frac{\partial z^{(0)}}{\partial \eta} &= 4Prx \frac{\partial z^{(0)}}{\partial x} \\ \text{with, } z^{(0)}(\eta, x) &= \begin{cases} 1 & \eta = +\infty \\ 0 & \eta = -\infty \end{cases} \end{aligned} \right\} \quad (89)$$

Upon comparing equation 89 with equation 85b it is obvious that

$$z^{(n)}(\eta, x) = F(\eta) \quad (90)$$

A basis for an iterative solution for the dimensionless temperature in a region in which chemical reaction is occurring is now available. In view of the fact that similar iterative solutions will be employed in Parts IV and V, in which combustion in the shear-flow mixing region and in the boundary layer are considered respectively, a rather detailed treatment of the iterative technique utilized throughout this paper will be presented at this time.

Define the following two dimensionless quantities.

$$\begin{aligned} \text{a) } Q^{(n)}(\eta, x) &= 4 \left[ \frac{1}{c_1 c_3} \frac{\partial z^{(n)}}{\partial x} + \theta_n^{(n)}(\eta, x) \right] \exp(R\eta^2) \\ \text{b) } X(x) &= c_1 c_3 x \end{aligned} \quad (91)$$

In the above, the symbol  $z^{(n)}(\eta, x)$  indicates the N'th approximation to the dimensionless temperature profile in a region in which chemical reaction is occurring. Correspondingly, the symbol  $\theta_n^{(n)}(\eta, x)$  represents  $\theta_n(\eta, x)$ , equation 60, evaluated with  $z(\eta, x)$  replaced by  $z^{(n)}(\eta, x)$ . If the right hand side of equation 85a is now approximated, using a known but approximate expression for  $z(\eta, x)$ , then the next higher approximation to  $z(\eta, x)$  may be obtained from the following partial differential equation which is based on equations 85a and 91.

$$\frac{\partial^2 z^{(N)}}{\partial \eta^2} + 2Pr\eta \frac{\partial z^{(N)}}{\partial \eta} = Pr \mathbb{I} Q^{(N-1)}(\eta, x) \exp(-Pr\eta^2)$$

with,

$$z^{(N)}(\eta, x) = \begin{cases} 1 & ; \eta = +\infty \\ 0 & ; \eta = -\infty \end{cases} \quad (92)$$

Equation 92 is fortunately of such a form that a general analytic solution can be obtained. The solution, which is carried out in Appendix B. 2, is as follows:

$$z^{(N)}(\eta, x) = F(\eta) - \mathbb{I}(x) \bar{z}^{(N-1)}(\eta, x) \quad (93)$$

where,

$$(a) \quad \bar{z}^{(N-1)}(\eta, x) = [F(\eta) R^{(N-1)}(\infty, x) - R^{(N-1)}(\eta, x)]$$

$$(b) \quad R^{(N-1)}(\eta, x) = \int_{-\infty}^{\eta\sqrt{Pr}} [e^{-\theta^2} \mathcal{L}^{(N-1)}(\theta, x)] d\theta \quad (94)$$

$$(c) \quad \mathcal{L}^{(N-1)}(\theta, x) = \int_0^{\theta\sqrt{Pr}} Q^{(N-1)}\left(\frac{\alpha}{\sqrt{Pr}}, x\right) d\alpha$$

From equations 91a and 60 respectively,

$$(a) \quad Q^{(N-1)}\left(\frac{\eta}{\sqrt{R}}, x\right) = 4e^{\eta^2} \left[ \frac{1}{c_1 c_3} \frac{\partial z^{(N-1)}\left(\frac{\eta}{\sqrt{R}}, x\right)}{\partial x} + \theta_2^{(N-1)}\left(\frac{\eta}{\sqrt{R}}, x\right) \right]$$

where,

$$(b) \quad \theta_2^{(N-1)}\left(\frac{\eta}{\sqrt{R}}, x\right) = \left[ 1 - 2c_2 z^{(N-1)}\left(\frac{\eta}{\sqrt{R}}, x\right) \right]^{1-m^*} \prod_{j=1}^{m^*} K_j^{(N-1)}\left(\frac{\eta}{\sqrt{R}}, x\right) \cdot \exp\left[ \frac{-\beta_1}{1 - 2c_2 z^{(N-1)}\left(\frac{\eta}{\sqrt{R}}, x\right)} \right]$$

(95)

The corresponding approximations for the species weight fractions and for the mixture density are obtained from equations 86 and 93:

$$(a) \quad K_i^{(N)}(\eta, x) = K_{i,II} + \Delta_i F(\eta) - \frac{1}{c_i} \mathfrak{X}(x) Z^{(N-1)}(\eta, x) \quad i \leq m^*$$

$$(b) \quad K_d(\eta, x) = K_{d,II} + \Delta_d F(\eta)$$

$$(c) \quad K_p^{(N)}(\eta, x) = K_{p,II} [1 - F(\eta)] + \frac{m^*}{c_1} \mathfrak{X}(x) Z^{(N-1)}(\eta, x)$$

$$(d) \quad S^{(N)}(\eta, x) = \frac{\rho M}{\mathcal{R} T^{(N)}(\eta, x)} \quad ; \quad T^{(N)}(\eta, x) = T_{II} - (T_{II} - T_I) z^{(N)}(\eta, x)$$

(96)

One additional relation, also obtained in Appendix B. 2, will be useful in later considerations of the "flame attachment distance".

$$\frac{\partial z^{(N)}}{\partial \eta} = \left\{ \sqrt{\frac{P_r}{\pi}} \left[ 1 - \Sigma(x) R^{(N-1)}(\infty, x) \right] + \sqrt{P_r} \Sigma(x) z^{(N-1)}(\eta, x) \right\} \exp(-P_r \eta^2) \quad (97)$$

The complete N'th approximation to the solution for the shear-free mixing region with first-order, second-order, or third-order chemical reaction is explicitly given in equations 93 through 97. Particular, and simpler, expressions for the first approximation will now be obtained; the first approximation will normally be sufficient for the purposes of an exploratory investigation such as the present study.

From equations 86a and 90 it follows that:

$$K_{z_i}^{(e)}(\eta, x) = K_{z_i}^{(e)}(\eta) = K_{z_i} + \Delta_{z_i} F(\eta) \quad (98)$$

Setting  $N = 1$  in equation 95a, and utilizing equations 90, 95b, and 98:

$$(a) \quad Q(\eta) \equiv Q^{(e)}\left(\frac{\eta}{\sqrt{P_r}}, x\right) = 4 \left[ 1 - 2c_2 \bar{F}(\eta) \right]^{1-m^*} \cdot \prod_{j=1}^{m^*} \left[ K_{z_{jI}} + \Delta_{z_j} \bar{F}(\eta) \right] \exp \left[ \eta^2 - \frac{\beta_j}{1 - 2c_2 \bar{F}(\eta)} \right] \quad (99)$$

where from equation 88,

$$(b) \quad \bar{F}(\eta) \equiv F\left(\frac{\eta}{\sqrt{P_r}}\right) = \frac{1}{2} (1 + \operatorname{erf} \eta)$$

From equations 94 and 99,

$$\begin{aligned}
 (a) \quad Z(\eta) &\equiv Z^{(0)}(\eta, x) = [F(\eta)R(\infty) - R(\eta)] \\
 (b) \quad R(\eta) &\equiv R^{(0)}(\eta, x) = \int_{-\infty}^{\eta\sqrt{P_r}} e^{-\eta^2} Z(\eta) d\eta \\
 (c) \quad Z(\eta) &\equiv Z^{(0)}(\eta, x) = \int_0^{\eta\sqrt{P_r}} Q(x) dx
 \end{aligned}
 \tag{100}$$

The first-approximation to the dimensionless temperature in a region in which chemical reaction is occurring is obtained upon substituting equation 100 into equation 93.

$$Z^{(1)}(\eta, x) = F(\eta) - X(x)Z(\eta)
 \tag{101}$$

The first-approximations to the species concentrations and to the mixture density are obtained from equation 96 upon setting  $N = 1$  and utilizing equation 100:

$$\begin{aligned}
 (a) \quad K_{i, \text{II}}^{(1)}(\eta, x) &= K_{i, \text{II}} + \Delta_i F(\eta) \frac{1}{c_i} X(x)Z(\eta) \quad ; \quad i \leq m^* \\
 (b) \quad K_d(\eta, x) &= K_{d, \text{II}} + \Delta_d F(\eta) \\
 (c) \quad K_p^{(1)}(\eta, x) &= K_{p, \text{II}} [1 - F(\eta)] + \frac{m^*}{c_i} X(x)Z(\eta) \\
 (d) \quad \rho^{(1)}(\eta, x) &= \frac{\rho M}{RT^{(1)}(\eta, x)} \quad ; \quad T^{(1)}(\eta, x) = T_{\text{II}} - (T_{\text{II}} - T_{\text{I}}) Z^{(1)}(\eta, x)
 \end{aligned}
 \tag{102}$$



Finally, from equations 97 and 100,

$$\left. \frac{\partial z^{(i)}}{\partial \eta} = \left\{ \sqrt{\frac{P_r}{\pi}} \left[ 1 - \mathbf{X}(x) R(\infty) \right] + \sqrt{P_r} \mathbf{X}(x) \mathcal{L}(\eta) \right\} e^{-P_r \eta^2} \right] \quad (103)$$

From equation 103 it follows that,

$$\left. \begin{array}{l} \text{a) } \eta = \pm \infty \\ \text{b) } \mathbf{X}(x) = \left[ R(\infty) - \sqrt{\pi} \mathcal{L}(\eta) \right]^{-1} \end{array} \right] \quad \text{When: } \frac{\partial z^{(i)}}{\partial \eta} = 0 \quad (104)$$

Equation 104a is simply a statement of the required boundary conditions on the temperature derivative with respect to  $\eta$ . Equation 104b defines the value of  $\mathbf{X}(x)$  as a function of  $\eta$  for which a temperature bulge exists; it thus defines the line in the  $\eta, x$  plane along which the temperature is maximum. The value of  $\eta$  which corresponds to the minimum value of  $\mathbf{X}(x)$  at which a temperature bulge exists is obtained from the following relation; cf. equations 100c and 104b.

$$\left. \frac{d}{d\eta} \left[ R(\infty) - \sqrt{\pi} \mathcal{L}(\eta) \right]_{\eta=\eta_i}^{-1} = \frac{-\sqrt{\pi} Q(\eta_i \sqrt{P_r})}{\left[ R(\infty) - \sqrt{\pi} \mathcal{L}(\eta) \right]^2} = 0 \right] \quad (105)$$

In the above equation,  $\eta_i$  denotes the value of  $\eta$  for which equation 105 is satisfied.

Now for at least one of the active reactant species ( $1 \leq i \leq m^*$ ),  $K_{i, \mathbf{I}}$  will be equal to zero; thus at least one of the terms in the

product function of equation 99a will be given by  $1/2 (1 + \operatorname{erf} \eta \sqrt{Pr}) K_{i, \infty}$ . Equation 105 will then be satisfied when  $(1 + \operatorname{erf} \eta \sqrt{Pr}) = 0$ ; thus

$$\eta_i = -\infty \quad (106)$$

According to equation 106, a temperature bulge first occurs for  $\eta_i = -\infty$ . The temperature bulge then grows and moves in the  $\eta, x$  plane in accordance with equation 104b. This conclusion is somewhat different from the result of the perturbation analysis of Marble and Adamson. According to their numerical calculations, a temperature bulge first occurs for a value of  $\eta_i$  of approximately  $-3.25^*$ . Their result is based on the numerical solution of an equation involving the first perturbation term; because of the asymptotic nature of the function  $f'(\eta)$  which occurs in this equation, it is not surprising that a large (finite) negative value of  $\eta_i$  was calculated as compared to the present result of negative infinity. A verification of the result of the present analysis can readily be obtained from the N'th approximation, equation 97, using the same technique employed for the first-approximation. In the region of initial chemical reaction, it can also be shown that the integrand of the reaction integral, equation 99a, is maximum at  $\eta_i = -\infty$ ; the initial temperature bulge would be expected to occur where the reaction integrand is at a maximum.

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\* The value of  $\eta$  as defined in the present analysis (cf. equation 74) is one-half that as defined by Marble and Adamson. The present definition was introduced in order that the definition of  $\eta$  for the mixing region case would be the same as the definition commonly employed in the boundary layer case.

The mathematical interpretation of an initial temperature bulge at  $\eta_{\lambda} = -\infty$  is that the initial bulge occurs when  $x_0 = 0$  at an indeterminate value of  $y_0$ . Since the diffusion velocity of active chemical species from the upper to the lower stream is finite, the concentration of these species in the lower stream at  $x_0 = 0$  is zero except at  $y_0 = 0$ ; the value of  $\eta_{\lambda}$  at this point is mathematically indeterminate, but could be  $-\infty$ . From physical considerations it thus appears that the initial temperature bulge must occur at the origin where mixing is initiated. The initial preponderant effect of the Arrhenius factor in the reaction integral will then rapidly pull the temperature bulge deep into the lower stream for increasing values of  $x_0$ ; finally, however, the scarcity of chemically active species from the upper stream will force the temperature bulge to move back toward the upper stream. The isotherm field will thus be similar to that presented in figure 3. The line of maximum temperature, along which equation 104b is satisfied, is indicated by the dashed line.

A "characteristic flame attachment length", denoted by  $x^*$  will be arbitrarily defined as the value of  $x$  at which the line of maximum temperature crosses the line  $\eta = -3.00$ . Thus from equation 91b and 104b:

$$\Sigma^*(x) = C_1 C_3 x^* = [R(\infty) - \sqrt{\pi} \mathcal{L}(-3.0)]^{-1} \quad (107)$$

The characteristic length could be defined in other ways. Any definition, however, would be equally arbitrary. The present definition is in reasonably good quantitative agreement with that of Marble and

Adamson; furthermore, calculations indicate that the heat release normally becomes significant in the region where  $\eta = -3.0$  and  $\partial z/\partial \eta = 0$ . Equation 107 thus defines the streamwise distance  $x^*$  at which the heat release due to chemical reaction first becomes significant.

It will usually be convenient to consider a "characteristic stay time" rather than the "characteristic flame attachment length". Define,

$$t^* = \frac{\lambda^*}{u_x} \quad (108)$$

Then from equations 47, 107, and 108:

$$t^* = \frac{(P/R T_x)^{1-m^*}}{bc_1 [R(\infty) - \sqrt{\pi} \mathcal{E}(-3.0)]} \quad (109)$$

Note that the stay time is independent of the velocity of the upper stream; the characteristic length is thus directly proportional to the velocity of the upper stream.

The complete first approximation to the general solution for the shear-free mixing region with chemical reaction is explicitly given in equations 99 - 102 and 109. Particular solutions for first-order, second-order, and third-order reactions can be obtained upon evaluating equation 99 using the appropriate value of  $m^*$  (the order of the reaction), and then evaluating the integrals in equation 100. Particular solutions for first-order and for second-order reactions are carried out in the following two sections.

C. Detailed Solution for First-Order Kinetics

In the case of first-order kinetics, the upper stream which is at temperature  $T_I$ , cf. sketch on page 65, will consist of a cold mixture of an exothermically decomposable fuel\* denoted by the subscript f, and an inert diluent gas, denoted by the subscript d. The lower stream, at temperature  $T_{II}$ , will consist of a hot inert gas, also denoted by the subscript d. If desired, the inert gases in the initial streams can be replaced by the product of combustion without affecting the following analysis †. In the mixing region, the gas mixture will thus consist of three components, fuel, combustion product, denoted by the subscript p, and inert diluent. The boundary conditions on the specie weight fractions are as follows:

At the cold boundary,  $\eta = +\infty$ :

At the hot boundary,  $\eta = -\infty$ :

$$K_{fI} = 1 - \epsilon$$

$$K_{dI} = \epsilon$$

$$K_{pI} = 0$$

$$K_{fII} = 0$$

$$K_{dII} = 1$$

$$K_{pII} = 0$$

(110)

\* Note that although the cold combustible stream at temperature  $T_I$  has been implicitly assumed to undergo chemical reaction only after the initiation of mixing ( $x_0 \geq 0$ ) the exponential variation of the reaction rate with temperature, equation 60, does not predict this zero value for  $x_0 < 0$ . Fortunately, however, the exponential variation does predict a rate of reaction at temperature  $T_I$  which is small enough to be neglected. This problem of the cold boundary condition is discussed by von Kármán and Millan in reference 5.

† In the case of an unopposed reaction, such as is being considered, the product specie is in effect an inert chemical specie; this is not true, of course, in the case of an opposed reaction.

In the above equation,  $\epsilon$  denotes the weight fraction of inert diluent present in the combustible stream. From equations 67b and 110:

$$\Delta_f = 1 - \epsilon \quad ; \quad \Delta_d = -(1 - \epsilon) \quad ; \quad \Delta_p = 0 \quad (111)$$

Equation 99a assumes a particularly simple form in the case of a first-order reaction, for in this case  $m^* - 1 = 0$ . Noting that there is but one term in the product function of equation 99a, namely the term for  $j = f$ , and substituting equations 99b, 110, and 111 into equation 99a, the following expression is obtained:

$$a) \quad Q(\eta) = (1 - \epsilon) \bar{Q}(\eta)$$

where:

(112)

$$b) \quad \bar{Q}(\eta) = 2(1 + \operatorname{erf} \eta) \exp\left[\eta^2 - \frac{\beta_1}{1 - c_2(1 + \operatorname{erf} \eta)}\right]$$

Now, using equation 107, define the following dimensionless independent variable:

$$\lambda \equiv \frac{\bar{X}(x)}{\bar{X}^*(x)} = \frac{x}{x^*} = \bar{X}(x) \left[ R(\infty) - \sqrt{\pi} \mathcal{L}(-3.0) \right] \quad (113)$$

The temperature and concentration profiles for two similar reacting flow systems having different values for the system parameters may be completely dissimilar for a given value of  $x$ ; the profiles will, however, be similar for a given value of  $\lambda$ ; cf. figures 4 and 6. The variable  $\lambda$  is indicative of the completeness of the reaction; it is a

more useful independent variable than the variable  $x$  which it replaces.

The following relations are obtained using equations 100, 101, 112, and 113:

$$a) \quad \mathcal{Z}^{(1)}(\eta, z) = F(\eta) - \mathcal{Z} \bar{Z}(\eta)$$

where,

$$b) \quad \bar{Z}(\eta) = \left[ \frac{F(\eta) \bar{R}(\infty) - \bar{R}(\eta)}{\bar{R}(\infty) - \sqrt{\pi} \bar{\mathcal{Z}}(-3.0)} \right]$$

$$c) \quad \bar{R}(\eta) \equiv \frac{R(\eta)}{1-\epsilon} = \int_{-\infty}^{\eta\sqrt{Pr}} e^{-\delta^2} \bar{\mathcal{Z}}(\delta) d\delta$$

$$d) \quad \bar{\mathcal{Z}}(\delta) \equiv \frac{\mathcal{Z}(\delta)}{1-\epsilon} = \int_0^{\eta\sqrt{Pr}} \bar{Q}(\alpha) d\alpha$$

$$e) \quad F(\eta) = \frac{1}{2} (1 + \operatorname{erf} \eta\sqrt{Pr})$$

(114)

The first-approximations to the specie concentrations and the mixture density are obtained from equations 102, 110, 111, and 113:

$$\begin{aligned}
 \text{a)} \quad K_f^{(1)}(\eta, z) &= (1-\epsilon)F(\eta) - \frac{z}{c_1} \bar{z}(\eta) \\
 \text{b)} \quad K_d(\eta) &= 1 - (1-\epsilon)F(\eta) \\
 \text{c)} \quad K_p^{(1)}(\eta, z) &= \frac{z}{c_1} \bar{z}(\eta) \\
 \text{d)} \quad \rho^{(1)}(\eta, z) &= \frac{\rho M}{RT^{(1)}(\eta, z)} \quad ; \quad T^{(1)}(\eta, z) = T_{II} - (T_{II} - T_I) g^{(1)}(\eta, z)
 \end{aligned}
 \tag{115}$$

The following expression for the characteristic stay time is obtained upon setting  $m^* = 1$  in equation 109 and then utilizing equation 114c:

$$(1-\epsilon)t^* = \left\{ bc_1 \left[ \bar{R}(\infty) - \sqrt{\pi} \bar{z}(-3.0) \right] \right\}^{-1}
 \tag{116}$$

Once the integrals of equations 114c and 114d are evaluated, the numerical calculation of the first-approximations for the temperature and specie concentrations in the mixing region with chemical reaction is perfectly straightforward using equations 114a and 115. The integrals are expressed in a suitable form for numerical evaluation by Simpson's rule. The numerical evaluation of these integrals and the calculations for the temperature and concentration profiles are discussed in Appendix D. The physical constants used are approximately those for the first-order decomposition of azomethane (discussed in Section IID) and are based on the data of Adamson<sup>(63)</sup> and of Hirschfelder et al<sup>(64)</sup>.



Temperature profiles (for  $Pr = Sc$ ) as calculated from equation 114a are presented in figure 4; the development of the temperature bulge is clearly indicated. Similar profiles as calculated from the perturbation analysis of Marble and Adamson<sup>(8)</sup> with  $Pr = 0.91$  and  $Sc = 1.00$  are presented for comparison in figure 5. The discrepancies in the profiles as calculated from the Marble-Adamson analysis and from equation 114a are due to the difference in the Schmidt number in the two cases and to the inherent differences in the analysis.

Concentration profiles (for  $Pr = Sc$ ) as calculated from equations 115a and 115b are presented in figure 6. As is to be expected, the combustible weight fraction decreases and the product specie weight fraction increases with increasing  $\lambda$ . The variation of the characteristic stay time, as calculated from equation 116, with the hot stream and adiabatic flame temperatures is presented in figure 7. As the hot stream temperature decreases the characteristic stay time, and also the characteristic flame attachment length, increases enormously. As pointed out by Marble and Adamson, the fact that semi-infinite streams are considered makes it impossible to calculate a blowoff velocity; however, for low hot stream temperatures the characteristic stay time becomes very large and the related characteristic attachment length becomes so large as to exceed the physical dimensions of any practical apparatus. The exponential character of the curves of figure 7 indicates that the Arrhenius factor is the dominant term in the reaction. Note that for a first-order reaction, the characteristic stay time is independent of the static pressure, cf. equation 116, and is inversely

proportional to  $(1 - \epsilon)$  where  $\epsilon$  is the weight fraction of inert diluent in the combustible free stream.

The minimum streamwise distance at which a temperature  $25^{\circ}\text{C}$  in excess of the hot stream temperature is attained can be readily calculated from equations 113 and 114a. Typical results of such calculation are presented in figure 8. The dependence of this streamwise distance upon adiabatic flame temperature (or heat release per unit mass of combustible) is relatively insensitive compared to the dependence upon the hot stream temperature. One point as calculated from the Marble-Adamson analysis is presented for comparison; for  $T_{II} = 1050^{\circ}\text{K}$  and  $T_f = 1650^{\circ}\text{K}$ , the Marble-Adamson analysis yields a streamwise distance for a  $25^{\circ}\text{C}$  temperature rise almost double that obtained from the present analysis. This is consistent with the results presented in figure 5 which indicates that the present analysis predicts a more rapid development of the temperature profile than does the Marble-Adamson analysis. However, for combustion studies in which exponential functions are dominant, the results of the two analyses are in satisfactory quantitative agreement.

#### D. Detailed Solution for Second-Order Kinetics

In the case of a second-order reaction, the gas mixture in the mixing region will consist of four distinct chemical species, fuel, oxidizer, product specie, and an inert diluent specie. The fuel and oxidizer may be initially premixed in the cold stream or may be initially separated, the fuel in the cold stream and the oxidizer in the hot stream. The former situation is typical of that in ramjet and turbo-

jet afterburner combustors where a relatively cool premixed combustible stream mixes with hot gases in the wake of bluff body flame stabilizers. The latter situation in which the fuel and oxidizer are initially separated corresponds to a special case of the diffusion flame. Both of these problems can be readily treated within the framework of the present analysis. A brief discussion of each of these problems follows.

1. The Premixed Case

In the premixed case, the upper stream which is at temperature  $T_I$ , cf. sketch on page 65, will consist of a cold combustible mixture of fuel, denoted by the subscript f, oxidizer, denoted by the subscript o, and an inert diluent, denoted by the subscript d. The lower stream, at temperature  $T_{II}$ , will consist of a hot inert gas, also denoted by the subscript d. The comments made on page 82 with regard to the assumption that the combustible stream does not react at temperature  $T_I$  also apply in the present instance. The boundary conditions on the specie weight fractions are as follows.

At the cold boundary,  $\eta = +\infty$  :

$$K_{f_I} = \phi \left( \frac{1-\epsilon}{1+\phi} \right)$$

$$K_{o_I} = \left( \frac{1-\epsilon}{1+\phi} \right)$$

$$K_{p_I} = 0 \quad ; \quad K_{d_I} = \epsilon \quad ;$$

At the hot boundary,  $\eta = -\infty$  :

$$K_{f_{II}} = 0$$

$$K_{o_{II}} = 0$$

$$K_{p_{II}} = 0$$

$$K_{d_{II}} = 1$$

(117)

In the above expressions,  $\phi$  denotes the equivalence ratio of the combustible mixture. This useful function is defined as the ratio of the

actual value of the fuel-oxidizer ratio to the value of the fuel-oxidizer ratio for a stoichiometric mixture; thus,  $\phi = 1$  for a stoichiometric mixture,  $\phi < 1$  for a fuel-lean mixture, and  $\phi > 1$  for a fuel-rich mixture. For the simple reaction being considered, involving mechanically similar molecules,  $\phi = K_{f_x} / K_{o_x}$ . The symbol  $\epsilon$  denotes the weight fraction of inert diluent in the combustible stream.

From equations 67b and 117:

$$\left. \begin{aligned} \Delta_f &= \phi \left( \frac{1-\epsilon}{1+\phi} \right) & \Delta_p &= 0 \\ \Delta_o &= \left( \frac{1-\epsilon}{1+\phi} \right) & \Delta_d &= -(1-\epsilon) \end{aligned} \right\} \quad (118)$$

The appropriate expression for the integrand of the reaction integral is obtained by setting  $j$  equal to  $o$  and  $f$  in equation 99a and utilizing equations 99b, 117, and 118:

$$\left. \begin{aligned} \text{a)} \quad Q(\eta) &= \phi \left( \frac{1-\epsilon}{1+\phi} \right)^2 \bar{Q}(\eta) \\ \text{where} \\ \text{b)} \quad \bar{Q}(\eta) &= \left[ \frac{(1+\text{erf } \eta)^2}{1-c_2(1+\text{erf } \eta)} \right] \exp \left[ \eta^2 - \frac{\beta_1}{1-c_2(1+\text{erf } \eta)} \right] \end{aligned} \right\} \quad (119)$$

Define:

$$a) \quad \bar{R}(\eta) \equiv \frac{1}{\phi} \left( \frac{1+\phi}{1-\epsilon} \right) R(\eta, \phi) = \int_{-\infty}^{\eta\sqrt{Pr}} e^{-\alpha^2} \bar{Z}(\alpha) d\alpha$$

where,

$$b) \quad \bar{Z}(\eta) \equiv \frac{1}{\phi} \left( \frac{1+\phi}{1-\epsilon} \right)^2 \mathcal{Z}(\eta, \phi) = \int_0^{\eta\sqrt{Pr}} \bar{Q}(\alpha) d\alpha$$

(120)

Then, using equations 100 - 102, 113, and 119, the following expressions for the first-approximations to the temperature, specie concentrations, and mixture density are obtained.

$$a) \quad z^{(1)}(\eta, \lambda) = F(\eta) - \lambda \bar{Z}(\eta)$$

$$b) \quad K_f^{(1)}(\eta, \lambda) = \phi \left( \frac{1-\epsilon}{1+\phi} \right) F(\eta) - \frac{\lambda}{c_1} \bar{Z}(\eta)$$

$$c) \quad K_o^{(1)}(\eta, \lambda) = \left( \frac{1-\epsilon}{1+\phi} \right) F(\eta) - \frac{\lambda}{c_1} \bar{Z}(\eta)$$

$$d) \quad K_p^{(1)}(\eta, \lambda) = \frac{2\lambda}{c_1} \bar{Z}(\eta)$$

$$e) \quad K_d(\eta) = 1 - (1-\epsilon) F(\eta)$$

$$f) \quad S^{(1)}(\eta, \lambda) = \frac{\rho M}{R T^{(1)}(\eta, \lambda)} \quad ; \quad T^{(1)}(\eta, \lambda) = T_{II} - (T_{II} - T_I) z^{(1)}(\eta, \lambda)$$

where,

$$g) \quad \bar{Z}(\eta) = \frac{F(\eta) \bar{R}(\infty) - \bar{R}(\eta)}{\bar{R}(\infty) - \sqrt{Pr} \bar{Z}(-3.0)}$$

$$h) \quad F(\eta) = \frac{1}{2} (1 + \operatorname{erf} \eta \sqrt{Pr})$$

(121)

The temperature and concentration profiles, as calculated from the above expressions, for a laminar mixing region with a second-order chemical reaction are very similar to those for a first-order reaction; cf. figures 4 and 6.

The following expression for the characteristic stay time is obtained upon setting  $m^* = 2$  in equation 109 and then utilizing equation 120a:

$$\bar{p} (1-\epsilon)^2 t^* = \left\{ \frac{82.08 T_{II} \frac{(1+\phi)^2}{\phi}}{b c_1 [\bar{R}(\infty) - \sqrt{\pi} \bar{F}(-3.0)]} \right\} \quad (\text{atmos-secs}) \quad (122)$$

The functions  $\bar{R}(\infty)$  and  $\bar{F}(-3.0)$  are functions of the activation energy  $E$  and of the stream temperatures  $T_I$  and  $T_{II}$ ; cf. equations 120, 119, and 59. If all parameters other than the static pressure are held constant, it thus follows from equation 122 that:

$$\left( t_{\bar{p}}^* / t_{\bar{p}=1}^* \right) = 1/\bar{p} \quad (123)$$

If all parameters other than the weight fraction of inert diluent in the combustible stream are held constant, then:

$$\left( t_{\epsilon}^* / t_{\epsilon=a}^* \right) = \left( \frac{1-a}{1-\epsilon} \right)^2 \quad (124)$$

If all parameters (including  $T_{II}$ ) other than the equivalence ratio are held constant, then:

$$\left( t_{\phi}^* / t_{\phi=1}^* \right) = \frac{(1+\phi)^2}{4\phi} \quad T_{II} = \text{constant} \quad (125)$$

Finally, if  $T_{II} = T_{II}(\phi)$  and all other parameters are held constant, then:

$$(t_{\phi}^* / t_{\phi=1}^*) = \frac{(1 + \phi)^2}{4\phi} \mathcal{J}(\phi) \quad ; \quad T_{II} = T_{II}(\phi) \quad (126)$$

where from equations 122 and 59:

$$\mathcal{J}(\phi) = \frac{\left\{ \left( \frac{T_f - T_x}{T_x - T_x} \right) [\bar{R}(\infty) - \sqrt{\pi} \bar{\mathcal{J}}(-3.0)] \right\}_{\phi=1}}{\left\{ \left( \frac{T_f - T_x}{T_x - T_x} \right) [\bar{R}(\infty) - \sqrt{\pi} \bar{\mathcal{J}}(-3.0)] \right\}_{\phi}} \quad (127)$$

If equations 119 and 120 are substituted into equation 127 and the resulting expression is then considerably simplified, using numerical calculations as a guide, the following simple relation is obtained as a satisfactory approximation to equation 127:

$$\mathcal{J}(\phi) \doteq \exp \left\{ \frac{E}{R T_x(\phi=1)} \left[ \frac{T_x(\phi=1)}{T_x(\phi)} - 1 \right] \right\} \quad (128)$$

Equations 123 through 126 and the functional forms of equations 123 and 128 are not restricted to the problem of the present analysis, combustion in the premixed shear-free laminar mixing region; identical or similar relations are obtained in the case of the shear-flow laminar mixing region (Part IV) and in the case of the laminar boundary layer (Part V). The pressure dependence, equation 123, is a direct result of the assumed law of mass action, equation 21, and is valid whenever this law is a satisfactory approximation to reality. The dependence upon the extent of vitiation, equation 124, is also of general applicability.

However, the dependence upon equivalence ratio, as given in equation 127, is strongly dependent upon the model employed for the mixing region problem. Since, for purposes of exploratory investigation, the present mixing region model is a satisfactory model for bluff body flame stabilizers, it might be expected that equations 122 through 128 would be in qualitative agreement with experimental data from experimental flame stabilization studies. In fact, surprisingly good quantitative agreement with experimental data is also obtained. This agreement, of course, is largely due to the fact that dimensionless ratios rather than absolute values are correlated: thus where the analysis might yield absolute quantities considerably in error, the ratio of two quantities which differ only due to the variation of a single parameter is in excellent agreement with experimental data. Some of the correlations with experimental data will be briefly discussed in the following paragraphs .

Mullins<sup>(65)</sup> has made measurements of the ignition delay of kerosene-air mixtures as a function of static pressure over the pressure range of 0.3 to 1.0 atmospheres. It was found that at a given free stream temperature the ignition delay varied essentially as the inverse of the static pressure. Since it is generally believed that the reaction between kerosene and air obeys second-order kinetics, and since the characteristic stay time of the present analysis is in effect an ignition delay time, Mullins' experimental measurements are in good agreement with the pressure dependence indicated by equation 123.

Zukoski<sup>(66)</sup> has determined that for a wide range of flow velocities and static pressures, the length of the recirculation zone



behind a bluff body flame stabilizer is essentially constant. Taking this length as a characteristic length and dividing by the blowoff velocity, a characteristic stay time for bluff body flame stabilization can be obtained. If the blowoff data of DeZubay<sup>(67)</sup> is reduced to the dependence upon static pressure of the ratio of the characteristic stay time at an arbitrary static pressure to that at one atmosphere, very satisfactory correlation with the pressure dependence indicated by equation 123 and with the data of Mullins is obtained; cf. figure 9.

The variation of the characteristic stay time with the weight fraction of inert diluent in the combustible stream as predicted by the present analysis is given in equation 124. In order to compare the results of the present analysis with the results of the experimental studies of Mullins<sup>(68)</sup> which are concerned with combustion in vitiated air, it will be convenient to introduce the "oxygen index"  $\alpha$  which he utilizes. This quantity is defined as the volumetric fraction of oxygen present in the vitiated air. The vitiated air consists essentially of oxygen, nitrogen, water vapor, and carbon dioxide. Since Mullins shows that the equivalent molecular weight of the vitiated air is relatively insensitive to the amount of vitiation and is close to that of oxygen, the oxygen index may be set equal to the weight fraction (rather than the volumetric fraction) of oxygen present in the vitiated air with little error. The combustible mixture will consist essentially of fuel, oxygen, and inert diluent. Thus:

$$\begin{aligned} K_o + K_f + \epsilon &= 1 \\ \alpha &= \frac{K_o}{K_o + \epsilon} \end{aligned}$$

]

(129)

The stoichiometric reaction of kerosene, the fuel used by Mullins, with oxygen is as follows:



The stoichiometric fuel-oxygen weight ratio is thus:

$$(f/o)_s = \frac{(1)(12) + (1)(2)}{(\frac{3}{2})(32)} = 0.292$$

It follows, therefore, that:

$$K_f = \phi (f/o)_s K_o = 0.292 \phi K_o \quad (130)$$

The following expression can be obtained upon combining equations 129 and 130.

$$\epsilon = \left[ 1 + \frac{\alpha}{1-\alpha} (1 + 0.292\phi) \right]^{-1} \quad (131)$$

The variation of the inert diluent weight fraction with the oxygen index and the equivalence ratio is presented in figure 10; note that  $\alpha = 0.21$  corresponds to unvitiated air while lower values of  $\alpha$  correspond to vitiated air. If equation 131 is substituted into equation 124, the following expression can be obtained

$$\left( t_{\alpha}^* / t_{\alpha=0.21}^* \right) = \left( \frac{0.21}{\alpha} \right)^2 \left[ \frac{1 + 0.0613\phi}{1 + 0.292\alpha\phi} \right]^2 \quad (132)$$

The variation of the characteristic stay time with the oxygen index as predicted by equation 131 is given by the three solid line curves in

figure 11. Mullins<sup>(68)</sup> correlated his experimental data and concluded that,

$$\left( t_{\alpha}^* / t_{\alpha=0.21}^* \right) = \left( \frac{0.21}{\alpha} \right)^2 \quad ; \quad (\text{Mullins}) \quad (133)$$

a relation which is in very close agreement with equation 132. The empirical correlation of Mullins, equation 133, is given by the dashed line in figure 11. The equivalence ratio at which Mullins obtained his data cannot be determined from his published papers. However, as indicated by figure 11, the agreement of the present analysis with the empirical data of Mullins is satisfactory regardless of the experimental value of his equivalence ratio.

The variation of the characteristic stay time with equivalence ratio in the simple case in which  $T_{II} = \text{constant}$ , equation 125, is presented in figure 12. In applying the results of the present analysis to bluff body flame stabilizers, however, it is apparent that the hot stream of the simple model of the sketch on page 65 will correspond to the hot recirculation zone behind the bluff body; thus  $T_{II} = T_{II}(\phi)$  is given by the wake temperature. Zukoski<sup>(66)</sup> has measured wake temperatures as a function of equivalence ratio. If his experimental values of wake temperature are utilized for the function  $T_{II} = T_{II}(\phi)$  in equation 128, and an activation energy of 43 kcals/g-mole (also estimated from experimental data of Zukoski) is utilized, the stay times can be calculated from equations 126 and 128. Zukoski has also measured the length of the recirculation zone at blowoff as a function

of the equivalence ratio; upon dividing this length by the corresponding blowoff velocity he obtained the characteristic stay time as a function of the equivalence ratio. The agreement between the experimentally measured dependence of the characteristic stay time upon equivalence ratio and the calculated dependence is quite good; cf. figure 13. It should be noted that the same functional relations (equations 125, 126, and 128) are found regardless of the stream velocity ratio; the fact that Zukoski's experimental points, figure 13, are for different values of the stream velocity ratio does not invalidate the agreement with the theoretical curve which is valid for all values of the velocity ratio.

The functional relations of the present analysis predict the variation of the characteristic stay time (or equivalently, of the blowoff velocity) with static pressure, extent of vitiation, and equivalence ratio, with surprising consistency with available experimental data. The application of such functional relations may reduce the amount of experimental data which must be obtained in developing turbojet afterburner combustors or other technologically important combustion devices.

## 2. The Diffusion Flame

In the case of the diffusion flame, the upper stream which is at temperature  $T_I$ , cf. sketch on page 65, will consist of a cold mixture of fuel and of inert diluent. The lower stream, at temperature  $T_{II}$ , will consist of a hot mixture of oxidizer and inert gas. The boundary conditions on the specie weight fractions are as follows:

At the cold boundary,  $\eta = +\infty$  :

At the hot boundary,  $\eta = -\infty$  :

$$K_{f_I} = 1 - \epsilon_I$$

$$K_{f_{II}} = 0$$

$$K_{o_I} = 0$$

$$K_{o_{II}} = 1 - \epsilon_{II}$$

$$K_{p_I} = 0$$

$$K_{p_{II}} = 0$$

$$K_{d_I} = \epsilon_I$$

$$K_{d_{II}} = \epsilon_{II}$$

(134)

The mass rate of fuel flow per unit cross-sectional area of the upper stream is given by:

$$\dot{m}_f = K_{f_I} \rho_I u_I = (1 - \epsilon_I) \rho_I u_I$$

Similarly, the mass rate of oxidizer flow per unit cross-sectional area of the lower stream is given by:

$$\dot{m}_o = K_{o_{II}} \rho_{II} u_{II} = (1 - \epsilon_{II}) \rho_{II} u_{II} \Lambda$$

The equivalence ratio is thus given by:

$$\phi = \dot{m}_f / \dot{m}_o = \left( \frac{1 - \epsilon_I}{1 - \epsilon_{II}} \right) \left( \frac{T_{II}}{T_I} \right) \frac{1}{\Lambda}$$

(135)

From equations 67b, 134, and 135:

$$\Delta_f = (1 - \epsilon_I)$$

$$\Delta_o = - \frac{(1 - \epsilon_{II})}{\phi} \left( \frac{T_{II}}{T_I} \right) \frac{1}{\Lambda}$$

$$\Delta_p = 0$$

$$\Delta_d = (1 - \epsilon_I) \left[ \frac{T_{II}}{T_I} \frac{1}{\phi \Lambda} - 1 \right]$$

(136)

Now define

$$\epsilon = \frac{\epsilon_I + \epsilon_{II}}{2} \quad (137)$$

the overall weight fraction of inert diluent in the flow system. From equations 135 and 137:

$$(1 - \epsilon_I) = \left[ \frac{2\phi\Lambda(1-\epsilon)}{\phi\Lambda + T_{II}/T_I} \right] \quad (138)$$

From equations 134, 135, 136, and 138, setting  $j$  equal to 0 and  $f$ :

$$\prod_{j=1}^2 [K_{\lambda_{II}} + \Delta_{\lambda} \bar{F}(\eta)] = \left\{ \bar{F}(\eta) [1 - \bar{F}(\eta)] \frac{4\phi(1-\epsilon)^2 (T_{II}/T_I)}{[\phi + \frac{1}{\Lambda}(T_{II}/T_I)]^2} \right\} \quad (139)$$

For the case presently under consideration, shear-free flow,  $\Lambda = 1$ .

The appropriate expression for the integrand of the reaction integral is obtained upon substituting equation 139 into equation 99a and utilizing equation 99b:

$$a) \quad Q(\eta) = \left\{ \frac{4\phi(1-\epsilon)^2 (T_{II}/T_I)}{[\phi + (T_{II}/T_I)]^2} \right\} \bar{Q}(\eta)$$

where,

$$b) \quad \bar{Q}(\eta) = \left[ \frac{1 - (\text{erf } \eta)^2}{1 - c_2(1 + \text{erf } \eta)} \right] \exp \left[ \eta^2 - \frac{\beta_1}{1 - c_2(1 + \text{erf } \eta)} \right]$$

(140)

Now define:

$$a) \quad \bar{R}(\eta) \equiv \left[ \frac{(\phi + T_{II}/T_I)^2}{4\phi(1-\epsilon)^2(T_{II}/T_I)} \right] R(\eta) = \int_{-\infty}^{\eta\sqrt{R}} e^{-\eta^2} \bar{\mathcal{L}}(\eta) d\eta$$

where,

$$b) \quad \bar{\mathcal{L}}(\eta) \equiv \left[ \frac{(\phi + T_{II}/T_I)^2}{4\phi(1-\epsilon)^2(T_{II}/T_I)} \right] \mathcal{L}(\eta) = \int_0^{\eta\sqrt{R}} \bar{Q}(\alpha) d\alpha$$

(141)

Using the above definitions, the temperature and concentration profiles and the characteristic stay time can be determined by direct substitution, into equations 121 and 122.

The dependence of the characteristic stay time upon static pressure and the overall weight fraction of inert diluent is identical with the premixed case; cf. equations 123 and 124. For a diffusion flame,  $T_{II}$  will not depend upon the equivalence ratio. The dependence of the characteristic stay time upon equivalence ratio can thus be simply obtained from equations 122 and 141; the integrals, being independent of  $\phi$ , cancel and the following simple relation, analogous to equation 125 for the premixed case, is obtained:

$$\left( t_{\phi}^* / t_{\phi=1}^* \right) = \frac{1}{\phi} \left[ \frac{\phi + T_{II}/T_I}{1 + T_{II}/T_I} \right]^2$$

(142)

This equation is valid only in the shear-free case,  $\Lambda = 1$ . A general expression valid when  $\Lambda \neq 1$  is obtained in Part IV.

IV. COMBUSTION IN THE SHEAR-FLOW LAMINAR MIXING REGION,  
STREAM VELOCITIES NOT EQUAL, WITH  $Pr = Sc$ :

A. The Velocity Field in the Shear-Flow Mixing Region

The formulation of the combustion problem in the shear-flow laminar mixing region ( $\Lambda \neq 1$ ) is exactly the same as the formulation presented in Section IIIA. The governing relations are presented in equation 82 for the case  $Pr = Sc \neq 1$ , and in equation 83 for the case  $Pr = Sc = 1$ . The corresponding boundary conditions on the differential equations are presented in equation 84.

In both of the cases noted above, the velocity field is given by the relations,

$$\begin{array}{l}
 \text{a) } \quad U = \frac{u - u_{II}}{u_I - u_{II}} = \frac{1}{2} f'(\eta) - \frac{\Lambda}{1 - \Lambda} \\
 \text{b) } \quad f'''(\eta) + f(\eta) f''(\eta) = 0 \\
 \text{c) } \quad f'(\eta) = \begin{cases} \frac{2}{1 - \Lambda} & ; \quad \eta = +\infty \\ \frac{2\Lambda}{1 - \Lambda} & ; \quad \eta = -\infty \end{cases}
 \end{array} \quad (143)$$

where  $\Lambda = u_{II}/u_I$  is the velocity ratio of the two streams prior to mixing. The differential equation with the associated boundary conditions can only be solved by numerical methods. Lock<sup>(57)</sup> and Görtler<sup>(58)</sup> have studied the solution to this problem. Lock numerically integrated the differential equations for the particular cases  $\Lambda = 0$  and  $\Lambda = 0.5$



starting from the analytic asymptotic expansions of the function and its derivatives. The ingenious solution of Görtler, being of general applicability for all values of  $\Lambda$ , is more useful in the present application. Görtler assumed a series solution of the following form:

$$f(\eta) = \sum_{m=0}^{\infty} \lambda^m g_m(\eta) \quad (144)$$

The series was then substituted into equation 143b, terms of the same power of  $\lambda$  were collected, and the resulting equations for the functions were solved. An analytic solution was obtained for  $g_1(\eta)$ ; all other  $g_m$ 's are evaluated by numerical integrations. The convergence of the series in  $g_m(\eta)$  is very rapid; the first two terms give sufficient accuracy for present purposes. If Görtler's solution for  $f(\eta)$  is differentiated with respect to  $\eta$  and equation 143a is utilized, the following expression for the velocity distribution is obtained:

$$U(\eta) = \frac{u - u_x}{u_z - u_x} = \left[ 1 + \operatorname{erf} \left( \eta \sqrt{\frac{1+\Lambda}{2(1-\Lambda)}} \right) \right]; \Lambda \neq 1 \quad (145)$$

Velocity profiles, as calculated from equation 145, are presented in figure 14.

#### B. General Solution for the Temperature and Concentration Fields in the Shear-Flow Mixing Region

The temperature field in the shear-flow mixing region can be obtained in the same manner as was the temperature field in the shear-free case; cf. Part III. Utilizing the same iterative technique as

previously employed, equations 82b, 83b, and 84 may be expressed as follows:

$$a) \quad \frac{\partial^2 z^{(N)}}{\partial \eta^2} + P_r f(\eta) \frac{\partial z^{(N)}}{\partial \eta} = \Sigma(x) Q^{(N-1)}(\eta, x) [f''(\eta)]^{P_r}$$

$$\text{with: } z^{(N)}(\eta, x) = \begin{cases} 1 & ; \eta = +\infty \\ 0 & ; \eta = -\infty \end{cases}$$

where,

$$b) \quad Q^{(N-1)}(\eta, x) = 2P_r \left\{ \frac{f'(\eta)}{C_1 C_3} \frac{\partial z^{(N-1)}}{\partial x} + 2\theta_{\sim}^{(N-1)}(\eta, x) \right\} [f''(\eta)]^{-P_r}$$

$$c) \quad \Sigma(x) = C_1 C_3 x$$

(146)

Equation 146a is fortunately of such a form that a general analytic solution can be obtained. The solution, which is carried out in Appendix B. 4, is as follows:

$$a) \quad z^{(N)}(\eta, x) = F(\eta) - \Sigma(x) Z^{(N-1)}(\eta, x)$$

where:

$$b) \quad Z^{(N-1)}(\eta, x) = [F(\eta) R^{(N-1)}(\infty, x) - R^{(N-1)}(\eta, x)]$$

$$c) \quad R^{(N-1)}(\eta, x) = \int_{-\infty}^{\eta} \left\{ [f''(\alpha)]^{P_r} Z^{(N-1)}(\alpha, x) \right\} d\alpha$$

$$d) \quad Z^{(N-1)}(\alpha, x) = \int_0^{\alpha} Q^{(N-1)}(\alpha, x) d\alpha$$

(147)

The function  $f''(\eta)$  can be obtained from equations 143a and 145:

$$f''(\eta) = 2 \frac{dU}{d\eta} = \exp\left[-\left(\frac{1+\Lambda}{1-\Lambda}\right)^2 \frac{\eta^2}{2}\right] \quad (148)$$

By virtue of the similarity solution for  $Pr = Sc = 1$ , (cf. Section II G. 2):

$$F(\eta) = U(\eta) \quad \text{when} \quad Pr = Sc = 1 \quad (149)$$

When  $Pr = Sc \neq 1$ , the function  $F(\eta)$  can be obtained upon solving the following partial differential equation; cf. equations 82c and 84:

$$\frac{\partial^2 F}{\partial \eta^2} + Pr f(\eta) \frac{\partial F}{\partial \eta} = 2 Pr x f'(\eta) \frac{\partial F}{\partial x}$$

with:

$$F(\eta, x) = \begin{cases} 1 & ; \eta = +\infty \\ 0 & ; \eta = -\infty \end{cases} \quad (150)$$

The form of equation 150 and the corresponding boundary conditions indicate that  $F(\eta, x) \equiv F(\eta)$ , thus

$$\frac{d^2 F}{d\eta^2} + Pr f(\eta) \frac{dF}{d\eta} = 0$$

$$F(\eta) = \begin{cases} 1 & \eta = +\infty \\ 0 & \eta = -\infty \end{cases} \quad (151)$$

The solution to equation 151, carried out in Appendix B. 3, is as follows:

$$F(\eta) = \frac{\int_{-\infty}^{\eta} [f''(\alpha)]^{Pr} d\alpha}{\int_{-\infty}^{\infty} [f''(\alpha)]^{Pr} d\alpha} \quad ; \quad Pr = Sc \neq 1 \quad (152)$$

Expressions for the concentrations of the various chemical species in the flow system can now be obtained by simple substitution of equations 147, 148, and 149 or 152 into the following expressions; cf. equations 82 and 83:

$$\begin{aligned}
 \text{a)} \quad K_i^{(N)} &= K_{i_{II}} + \frac{1}{c_i} (z^{(N)} - F) + \Delta_i F \quad ; \quad i \leq m^* \\
 \text{b)} \quad K_d &= K_{d_{II}} + \Delta_d F \\
 \text{c)} \quad K_p^{(N)} &= K_{p_{II}} (1-F) - \frac{m^*}{c_i} (z^{(N)} - F)
 \end{aligned}
 \tag{153}$$

### C. The Characteristic Stay Time

The following expression is derived in Appendix B. 4:

$$\frac{\partial z^{(N)}}{\partial \eta} = [f''(\eta)]^{Pr} \left\{ \frac{1 - \Sigma(x) R^{(N-1)}(\infty, x)}{\int_{-\infty}^{\infty} [f''(\alpha)]^{Pr} d\alpha} + \Sigma(x) \mathcal{L}^{(N-1)}(\eta, x) \right\}
 \tag{154}$$

Proceeding as in Part III, it is readily determined that the required condition for the occurrence of a temperature bulge in a shear-flow laminar mixing region is as follows:

$$\Sigma(x) = \left[ R^{(N-1)}(\infty, x) - \mathcal{L}^{(N-1)}(\eta, x) \int_{-\infty}^{\infty} [f''(\alpha)]^{Pr} d\alpha \right]^{-1}
 \tag{155}$$

The characteristic length and stay time are defined as in Part III.

The first approximation to the characteristic stay time is thus as follows:

$$t^* = \left\{ \frac{(\rho/R T_{II})^{1-m^*}}{bc_1 [R(\infty) - \mathcal{L}(-3.0) \int_{-\infty}^{\infty} [f''(\alpha)]^{Pr} d\alpha]} \right\} \quad (156)$$

As in Part III, it can easily be demonstrated (cf. equations 146a and 150) that,

$$z^{(0)}(\eta, x) = z^{(0)}(\eta) = F(\eta) \quad (157)$$

Then, from equations 60, 146b, and 157:

$$Q(\eta) \equiv Q^{(0)}(\eta, x) = 4Pr [1 - 2c_2 F(\eta)]^{1-m^*} \cdot \prod_{j=1}^{m^*} [K_{j,II} + \Delta_j F(\eta)] \exp\left[\frac{-\beta_1}{1 - 2c_2 F(\eta)}\right] \quad (158)$$

The variation of the characteristic stay time with the stream velocity ratio  $\Lambda$  can now be calculated using equations 145, 147-149, 152, 156, and 158. The calculations are straightforward, though rather lengthy, and will not be detailed in the present discussion. The variation of the characteristic stay time with the velocity ratio for the case where  $Pr = Sc = 1$  is presented in figure 15; the normalizing denominator  $(t_{\Lambda=1,0}^*)$  is calculated from equation 109, Part III. Figure 15 is in qualitative agreement with experimental studies of combustion in an axially symmetric mixing region by Wright<sup>(69)</sup>.

Following the procedure of Part III, the variation of the characteristic stay time with equivalence ratio in the case of a second-order chemical reaction occurring in a shear-flow laminar mixing region can be determined in a straightforward manner. When the fuel and oxidizer are initially premixed, the variation with equivalence ratio is identical with the shear-free case; cf. equations 125, 126, and 128. In the case of the diffusion flame, however, the variation is modified for velocity ratio:

$$\left( t_{\phi}^* / t_{\phi=1}^* \right) = \frac{1}{\phi} \left[ \frac{\phi + \frac{1}{\Delta} (\tau_{\text{B}} / \tau_{\text{F}})}{1 + \left( \frac{1}{\Delta} \right) (\tau_{\text{B}} / \tau_{\text{F}})} \right]^2 \quad (159)$$

Equation 159 can be validated using equations 134 - 136, 138, 147, 156, and 158. The functional relation of equation 159 is graphically portrayed in figure 16. The dependence upon the parameter  $(1/\Delta)(\tau_{\text{B}}/\tau_{\text{F}})$  is explained by the fact that as either the stream temperature or the velocity ratio changes, the relative mass rate of flow of fuel and oxidizer, and thus the equivalence ratio, also changes.

## V. COMBUSTION IN THE LAMINAR BOUNDARY LAYER OF A CONSTANT TEMPERATURE FLAT PLATE WITH $Pr = Sc$ :

### A. Formulation of the Combustion Problem in the Laminar Boundary Layer

Consider a semi-infinite steady gas stream flowing from left to right parallel to the  $x_0$  axis in the physical plane. The stream consists of a cold combustible gas mixture at temperature  $T_I$ , density  $\rho_I$ , and velocity  $u_I$ ; it is assumed that no chemical reaction takes place at temperature  $T_I^*$ . A semi-infinite flat plate extends along the positive half of the  $x_0$  axis. This plate is maintained at a constant temperature  $T_{II}$ , with  $T_I < T_{II} < T_f$  where  $T_f$  is the adiabatic flame temperature for a stoichiometric mixture of the free stream combustible constituents\*\*.

The free stream chemical concentrations will be specified and will serve as the mathematical boundary conditions along the cold boundary,  $\eta = \infty$ . The appropriate concentration boundary conditions along the hot boundary, the plate surface, are not as clearly evident. Two reasonable a priori possibilities exist: (1) the chemical concentrations along the plate surface may be specified, or (2) the concentration gradients along the plate surface may be set equal to zero.

In the first case where the concentrations along the wall are specified, the concentration gradients cannot be specified but must be

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\* See footnote page 82, and reference 5 for a discussion of this requirement on the cold boundary condition.

\*\* The general case in which the flat plate may assume an arbitrary temperature distribution is briefly discussed in Appendix F.

determined. Normally the gradients will be non-zero at the wall, indicating a net flux of a given chemical specie to or from the wall. A surface reaction corresponding to a destruction of those species which have a net flux to the wall and a production of those species which have a net flux from the wall must be assumed. Note that a net flux of a given chemical specie to or from the wall does not violate the law of conservation of mass at the wall nor does it require a distribution of mass sources or sinks along the wall. The absence of mass sources or sinks along the wall does not require that

$$\left. \frac{\partial K_i}{\partial \eta} \right|_{\eta=0} = 0 \quad \text{all } i$$

but rather only requires that,

$$\sum_i \left. \frac{\partial K_i}{\partial \eta} \right|_{\eta=0} = 0$$

a condition which is satisfied in the present analysis. Since the mass average velocity and the diffusion velocity are both very small near the wall, the stay time of a molecule very near the surface of the wall is large and it seems reasonable that while immersed in the hot layer near the wall, the molecule will react to form product species.

The second case, where the concentration gradients along the wall are set equal to zero, corresponds to the physical assumption that a molecule impinging on the wall rebounds as the identical specie



without chemical reaction; there is no net flux of any given chemical specie to or from the wall and thus a surface reaction need not be prescribed.

It is difficult to say a priori which of the two sets of concentration boundary conditions will serve as the best model for combustion within a laminar boundary layer of a constant temperature flat plate. The problem should be solved with both sets of conditions and the results compared for an a posteriori evaluation. Unfortunately the second case, of zero gradients at the wall, cannot be solved within the framework of the present similarity solution (Section II G) due to the similarity requirement that the concentrations as well as the temperature be specified constants along the plate surface; cf. equation 59. The specification of the concentrations along the cold boundary and the gradients along the hot boundary will complicate the analysis but should not render the problem intractable.

The present analysis, then, will be concerned only with the first case in which the concentrations are specified along the wall; the similarity solutions of Section II G may then be utilized. No claim as to the superiority of the boundary conditions of the first case as compared to those of the second case is made. Both cases should be solved but only the first case is compatible with the similarity solution of the present analysis. The results of the following analysis are, of course, only as valid as are the assumed boundary conditions.

The presence of the flat plate induces velocity and thermal boundary layers. Near the leading edge of the plate, the transfer of

heat to the combustible mixture within the thermal boundary layer initiates an exothermic chemical reaction which accelerates with increasing temperature. The increase in temperature is mutually provided by heat transfer from the plate and by the chemical reaction itself. The chemical reaction gains in intensity and in rate of heat release with the result that the local temperature finally exceeds the plate temperature. At this point the heat flux at the wall changes in sign and heat proceeds to flow from the thermal boundary layer to the plate rather than from the plate to the boundary layer as heretofore. The rate of chemical reaction, which is now substantial, is still increasing exponentially with the local temperature. At a very short distance downstream from the point at which the heat flux at the wall changes sign, therefore, a fully developed laminar flame front is established. Since the local flow velocity normal to the flame front is essentially equal to the flame propagating velocity, the flame front is almost normal to the plate deep within the boundary layer where the local flow velocity is very low, and then curves with a decreasing slope until it emerges from the boundary layer as a flat front lying at a shallow angle with respect to the free stream velocity vector. The curvature of the flame front is illustrated in figure 17a; lines of constant temperature, isotherms, are also presented. Note that the  $T_{II}$  isotherm is double branched and that all isotherms for temperatures from  $T_{II}$  to  $T_f$  are doubled valued functions in the physical plane. The value of the abscissa at which the  $T_{II}$  isotherm becomes double branched is denoted by the symbol  $x_o^*$ .

Typical temperature profiles at various downstream stations are presented in figure 17b. Note that as in the case of the mixing region, cf. Section III A, there is a zone near the leading edge of the plate in which the effects of chemical reaction are small and in which the chemical concentration and temperature fields differ only slightly from those of a boundary layer without chemical reaction. The iteration procedure utilized in the mixing region case can thus be applied in the boundary layer case; in the latter case, of course, the basis for the iteration will be the temperature profile for the flat plate with forced convection in the absence of chemical reaction.

In Section III A the restrictions on the applicability to the mixing region of the present analysis, which is based on the classic Prandtl boundary layer assumptions, were outlined. In particular, it was noted that with suitable restraints on the stream velocities, the boundary layer assumptions were valid throughout the entire mixing and flame zone regions. In the boundary layer case, however, the classic boundary layer assumptions always break down just downstream of the point at which the heat flux at the wall changes sign ( $x_0 > x_0^*$ ). No restraints on the initial stream conditions can be found, as in the mixing region case, which will validate the boundary layer assumptions throughout the entire flow field. The explanation for this fact is as follows: Regardless of the initial stream velocity, the flame front is almost normal to the plate deep within the boundary layer; since steep temperature gradients exist normal to the flame front, it follows that steep streamwise temperature gradients exist deep within the boundary

layer at the upstream end of the flame front. The existence of these steep streamwise temperature gradients violates the classic boundary layer assumptions.

In conclusion, the boundary layer analysis to be presented in the following four sections will be concerned only with the initial zone in which the reaction induced changes and the streamwise gradients in the physical variables are small; the classic boundary layer assumptions will thus be valid throughout the region of present interest regardless of the free stream flow velocity. Furthermore, as a consequence of the fact that the reaction induced variations are small in the region of interest, these variations may be treated as perturbations to the boundary layer without chemical reaction and an iterative solution for the boundary layer with chemical reaction may be obtained in a manner analogous with that employed in the mixing region case.

#### B. General Solution with $Pr = Sc$ :

The governing equations and corresponding boundary conditions for combustion in the laminar boundary layer with  $Pr = Sc$  are directly obtainable from equations 82 and 84. By virtue of the similarity solution for  $Pr = Sc$  (Section II B. 1) only three equations remain to be solved. The cold and hot boundaries in the  $\eta$ ,  $x$  plane of the analysis are  $\eta_I = \infty$  and  $\eta_{II} = 0$  respectively.

a)  $f'''(\eta) + f(\eta)f''(\eta) = 0$

with:  $f'(\eta) = \begin{cases} 2 & \eta = \infty \\ 0 & \eta = 0 \end{cases}$

b)  $\frac{\partial^2 z}{\partial \eta^2} + P_r f(\eta) \frac{\partial z}{\partial \eta} = 2 P_r x f'(\eta) \frac{\partial z}{\partial x} + 4 P_r X C_1 C_3 \theta_{\infty}(\eta, x)$

with:  $z(\eta, x) = \begin{cases} 1 & \eta = \infty \\ 0 & \eta = 0 \end{cases}$

c)  $\frac{\partial^2 F}{\partial \eta^2} + P_r f(\eta) \frac{\partial F}{\partial \eta} = 2 P_r x f'(\eta) \frac{\partial F}{\partial x}$

with:  $F(\eta, x) = \begin{cases} 1 & \eta = \infty \\ 0 & \eta = 0 \end{cases}$

(160)

The other unknowns are obtained upon substituting the solutions to the above equations into the following expressions from equation 82.

$$\begin{aligned}
 \text{a)} \quad K_{\lambda} &= K_{\lambda_{II}} + \Delta_{\lambda} F + \frac{1}{c_{\lambda}} (z - F) \quad ; \lambda \leq m^* \\
 \text{b)} \quad K_d &= K_{d_{II}} + \Delta_d F \\
 \text{c)} \quad K_p &= K_{p_{II}} (1 - F) - \frac{m^*}{c_1} (z - F) \\
 \text{d)} \quad U &= \frac{u}{u_{\infty}} = \frac{1}{2} f'(\eta) \\
 \text{e)} \quad \rho &= \frac{\rho M}{\rho T} \quad ; \quad T = T_{II} - (T_{II} - T_{\infty}) z
 \end{aligned} \tag{161}$$

Equation 160a has been solved by Blasius<sup>(60)</sup> using a numerical technique. A recent and more accurate numerical solution has been obtained by Emmions and Leigh<sup>(70)</sup> using modern high speed computing equipment. An excerpt from this work is presented in Table I.

The form of equation 160c and the corresponding boundary conditions indicate that  $F(\eta, x) \equiv F(\eta)$ , thus

$$\begin{aligned}
 \frac{d^2 F}{d\eta^2} + Pr f(\eta) \frac{dF}{d\eta} &= 0 \\
 \text{with: } F(\eta) &= \begin{cases} 1 & \eta = \infty \\ 0 & \eta = 0 \end{cases}
 \end{aligned} \tag{162}$$

The solution of equation 162 is obtained in Appendix B-3; the result is,

$$a) \quad F(\eta) = \mathcal{P}(\text{Pr}) \int_0^\eta [f''(\alpha)]^{\text{Pr}} d\alpha$$

where,

$$b) \quad \mathcal{P}(\text{Pr}) = \left[ \int_0^\infty [f''(\alpha)]^{\text{Pr}} d\alpha \right]^{-1} = \frac{0.664 \text{Pr}^{1/3}}{(1.328)^{\text{Pr}}}$$

(163)

The function  $\mathcal{P}(\text{Pr})$  is presented in figure 18.

The solution to equation 160b is not to be obtained so easily. However, as previously noted, this analysis is concerned with the initial region in which the reaction induced changes in the temperature are relatively small. A close approximation to the dimensionless temperature profile, namely that for the boundary layer without chemical reaction, can thus be obtained as a basis for an iterative solution. The dimensionless temperature for the boundary layer without chemical reaction, which will be denoted by the symbol  $z^{(0)}(\eta, x)$ , is given by equation 160b with the reaction term, the last term, set equal to zero. Thus,

$$\frac{\partial^2 z^{(0)}}{\partial \eta^2} + \text{Pr} f(\eta) \frac{\partial z^{(0)}}{\partial \eta} = 2 \text{Pr} x f'(\eta) \frac{\partial z^{(0)}}{\partial x}$$

with,

$$z^{(0)}(\eta, x) = \begin{cases} 1 & \eta = \infty \\ 0 & \eta = 0 \end{cases}$$

(164)

Upon comparing equations 160c and 164 it is obvious that

$$z^{(0)}(\eta, x) = F(\eta) \quad (165)$$

A basis for an iterative solution for the dimensionless temperature in a boundary layer region in which chemical reaction is occurring is now available. Now define the following two dimensionless quantities:

$$\begin{aligned} \text{a)} \quad Q^{(N)}(\eta, x) &= 2P_r [f''(\eta)]^{-Pr} \left\{ \frac{f'(\eta)}{C_1 C_3} \frac{\partial z^{(N)}}{\partial x} \right. \\ &\quad \left. + 2\Theta_2^{(N)}(\eta, x) \right\} \\ \text{b)} \quad X(x) &= C_1 C_3 x \end{aligned} \quad (166)$$

Proceeding as in the mixing region case, equations 160b and 166 can be combined to yield the following partial differential equation for the N'th approximation to the dimensionless temperature in a region in which chemical reaction is occurring.

$$\frac{\partial^2 z^{(N)}}{\partial \eta^2} + P_r f(\eta) \frac{\partial z^{(N)}}{\partial \eta} = [f''(\eta)]^{Pr} X(x) Q^{(N-1)}(\eta, x)$$

with, 
$$z^{(N)}(\eta, x) = \begin{cases} 1 & \eta = \infty \\ 0 & \eta = 0 \end{cases} \quad (167)$$

Equation 167 is fortunately of such a form that a general analytic solution can be obtained. The solution, which is carried out in



Appendix B-4 is as follows:

$$z^{(N)}(\eta, x) = F(\eta) - \bar{X}(x) z^{(N-1)}(\eta, x) \quad (168)$$

where,

$$a) \quad z^{(N-1)}(\eta, x) = [F(\eta) R^{(N-1)}(\omega, x) - R^{(N-1)}(\eta, x)]$$

$$b) \quad R^{(N-1)}(\eta, x) = \int_0^\eta \{ [f''(x)]^{Pr} z^{(N-1)}(x, x) \} dx \quad (169)$$

$$c) \quad z^{(N-1)}(\eta, x) = \int_0^x Q^{(N-1)}(x, x) dx$$

From equations 166a and 60 respectively,

$$a) \quad Q^{(N-1)}(\eta, x) = 2Pr [f''(\eta)]^{-Pr} \left\{ \frac{f'(\eta)}{c_1 c_3} \frac{\partial z^{(N-1)}}{\partial x} + 2 \theta_2^{(N-1)}(\eta, x) \right\}$$

where,

$$b) \quad \theta_2^{(N-1)}(\eta, x) = [1 - 2c_2 z^{(N-1)}(\eta, x)]^{1-m^*} \prod_{j=1}^{m^*} K_j^{(N-1)}(\eta, x) \cdot \exp \left[ \frac{-\beta_1}{1 - 2c_2 z^{(N-1)}(\eta, x)} \right] \quad (170)$$

The corresponding approximations for the species weight fractions and for the mixture density are obtained from equations 161 and 168:

$$\begin{aligned}
 \text{a)} \quad K_i^{(N)} &= K_{i_{\text{II}}} + \Delta_i F(\eta) - \frac{1}{c_i} \Sigma(x) Z^{(N-1)}(\eta, x) \quad ; \quad i \leq m^* \\
 \text{b)} \quad K_d(\eta, x) &= K_{d_{\text{II}}} + \Delta_d F(\eta) \\
 \text{c)} \quad K_p^{(N)}(\eta, x) &= K_{p_{\text{II}}} [1 - F(\eta)] + \frac{m^*}{c_i} \Sigma(x) Z^{(N-1)}(\eta, x) \\
 \text{d)} \quad \rho^{(N)}(\eta, x) &= \frac{\rho M}{R T^{(N)}(\eta, x)} \quad ; \quad T^{(N)}(\eta, x) = T_{\text{II}} - (T_{\text{II}} - T_{\text{I}}) Z^{(N)}(\eta, x)
 \end{aligned}
 \tag{171}$$

The following additional relation, also obtained in Appendix B-4, will be useful in considerations of a "characteristic stay time" for combustion in the laminar boundary layer.

$$\frac{\partial Z^{(N)}}{\partial \eta} = [F^0(\eta)]^{R'} \left\{ \rho(R) - \Sigma(x) \left[ \rho(R) R^{(N-1)}(\eta, x) - Z^{(N-1)}(\eta, x) \right] \right\}
 \tag{172}$$

In the preceding section it was noted that the classic boundary layer assumptions break down at the upstream end of the flame front

and that this upstream end normally occurs a short distance downstream of the point  $x_0 = x_0^*$  ( $x_0^*$  being defined as the value of the abscissa at which the  $T_{II}$  isotherm becomes double branched). An equivalent and more useful definition is that  $x_0^*$  is the length of the flat plate, measured from the leading edge, over which the heat flow is from the plate to the boundary layer; for  $x_0 > x_0^*$ , the heat flow is from the boundary layer to the plate. Since the plate is acting as a heat sink for  $x_0 > x_0^*$ , the substitution of a plate of finite length equal to  $x_0^*$  would be advantageous with regard to the stabilization of a flame within the laminar boundary layer of a constant temperature flat plate. It is thus observed that:  $x_0^*$  is the length of a finite flat plate at temperature  $T_{II}$  which is just sufficiently long to stabilize a flame within its laminar boundary layer. From this viewpoint, or the viewpoint that the flame attachment length (the length from the plate leading edge to the upstream end of the flame front) is just slightly greater than  $x_0^*$  and is not calculable from the present analysis because of the invalidity of the boundary layer assumptions in this region, the distance  $x_0^*$  may be taken as the fundamental characteristic length of the problem<sup>†</sup>.

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<sup>†</sup> The classic boundary layer assumptions are not valid at the upstream end of the flame front where the steep slope of the flame front in the boundary layer results in large streamwise temperature gradients. Just a short distance upstream, however, say at  $x_0 = x_0^*$ , the classic assumptions are valid; thus  $x_0^*$  can be calculated from the present analysis. The rapid change in  $x_0^*$  conditions in a short streamwise distance downstream of  $x_0^*$  is explained by the fact that the reaction rate is an exponential function of the local temperature; since the local temperature near the wall at  $x_0 = x_0^*$  is approximately equal to  $T_{II}$ , the reaction rate is high.

The preceding definition of  $x_0^*$  implies that,

$$\left. \frac{\partial z^{(N)}}{\partial \eta} \right|_{\substack{\eta=0 \\ x_0 = x_0^*}} = 0 \quad (173)$$

Thus, from equations 166b, 169c, 172, and 173:

$$X^{*(N)}(x) = c_1 c_3 X^{*(N)} = [R^{(N-1)}(\infty, x^{*(N)})]^{-1} \quad (174)$$

From equations 161, 165, 169, and 170:

$$\begin{aligned} \text{a)} \quad Q(\eta) &\equiv Q^{(0)}(\eta, x) = \left\{ \frac{4Pr [1 - 2c_2 F(\eta)]^{1-m^*}}{[f''(\eta)]^{Pr}} \right\} \cdot \\ &\quad \prod_{j=1}^{m^*} [K_{j_x} + \Delta_j F(\eta)] \exp \left[ \frac{-\beta_j}{1 - 2c_2 F(\eta)} \right] \\ \text{b)} \quad R(\eta) &\equiv R^{(0)}(\eta, x) = \int_0^\eta \left\{ [f''(x)]^{Pr} \mathcal{L}(x) \right\} dx \\ \text{c)} \quad \mathcal{L}(x) &\equiv \mathcal{L}^{(0)}(x, x) = \int_0^x Q(\omega) d\omega \end{aligned} \quad (175)$$

The "characteristic stay time" is defined as follows:

$$t^* = (x^*/u_x) \quad (176)$$

The first-approximation to the characteristic stay time is readily obtained from equations 60 and 174-176:

$$t_{(0)}^* = \left[ \frac{(P/RT_x)^{1-m^*}}{bc_1 R(\infty)} \right] \quad (177)$$

Now, using equations 174 and 175, define the following dimensionless independent variable:

$$\mathcal{R} \equiv \frac{\bar{X}^{(1)}(x)}{\bar{X}^{*(1)}(x)} = (X^{(1)}/X^{*(1)}) = \bar{X}(x) \mathcal{R}(\infty) \quad (178)$$

The temperature and concentration profiles for two similar reacting flow systems having different values for the system parameters may be completely dissimilar for a given value of  $x$ ; the profiles will, however, be similar for a given value of  $\mathcal{R}$ . The variable  $\mathcal{R}$  is indicative of the completeness of the reaction; it is a more useful independent variable than the variable  $x$  which it replaces.

The first-approximations to the temperature, specie concentrations, and mixture density can be readily obtained upon substituting equation 175 into the following expressions; cf. equations 168, 169a, 171, and 178:

$$\left. \begin{aligned} \text{a)} \quad z^{(1)}(\eta, \mathcal{R}) &= F(\eta) - \mathcal{R} \bar{z}(\eta) \\ \text{b)} \quad K_i^{(1)}(\eta, \mathcal{R}) &= K_{i\text{II}} + \Delta_i F(\eta) - \frac{\mathcal{R}}{c_1} \bar{z}(\eta) \quad ; i \leq m^* \\ \text{c)} \quad K_p^{(1)}(\eta, \mathcal{R}) &= K_{p\text{II}} [1 - F(\eta)] + \frac{m^* \mathcal{R}}{c_1} \bar{z}(\eta) \\ \text{d)} \quad K_d(\eta) &= K_{d\text{II}} + \Delta_d F(\eta) \end{aligned} \right\} (179)$$

$$e) \quad S^{(1)}(\eta, \nu) = \frac{P M}{R T^{(1)}(\eta, \nu)} \quad ; \quad T^{(1)}(\eta, \nu) = T_{II} - (T_{II} - T_I) z^{(1)}(\eta, \nu)$$

where,

$$f) \quad \bar{z}(\eta) \equiv \frac{\bar{z}^{(0)}(\eta, X)}{R(\infty)} = F(\eta) - \frac{R(\eta)}{R(\infty)}$$

(179  
cont'd)

The above expressions are valid when  $Pr = Sc$ . The particular and simpler case where  $Pr = Sc = 1$  will be considered in the following section.

C. Particular Solution for  $Pr = Sc = 1$ :

By virtue of the similarity solution for  $Pr = Sc = 1$ :

$$F(\eta) = U(\eta) = u/u_I = \frac{1}{2} f'(\eta) \quad ] \quad (180)$$

cf. equations 72 and 83f. The appropriate expressions for the first-approximation to the temperature, specie concentrations, mixture density and characteristic stay time are obtained upon substituting equation 180 into equations 175, 177, and 179:

$$a) \quad z^{(1)}(\eta, \nu) = \frac{1}{2} f'(\eta) - \nu \bar{z}(\eta)$$

$$b) \quad K_{i, \nu}^{(1)}(\eta, \nu) = K_{i, II} + \frac{1}{2} \Delta_i f'(\eta) - \frac{\nu}{c_i} \bar{z}(\eta) \quad ] \quad (181)$$

$i \leq m^*$

$$c) \quad K_d(\eta) = K_{d, II} + \frac{1}{2} \Delta_d f'(\eta)$$

$$\begin{aligned}
 \text{d)} \quad K_p^{(1)}(\eta, z) &= K_{p, \text{II}} \left[ 1 - \frac{1}{2} f'(\eta) \right] + \frac{m^* z}{c_1} \bar{z}(\eta) \\
 \text{e)} \quad S^{(1)}(\eta, z) &= \frac{pM}{RT^{(1)}(\eta, z)} \quad ; \quad T^{(1)}(\eta, z) = T_{\text{II}} - \\
 &\quad (T_{\text{II}} - T_{\text{I}}) z^{(1)}(\eta, z) \\
 \text{f)} \quad t^* &= \left\{ \frac{(p/RT_{\text{II}})^{1-m^*}}{bc_1 R(\infty)} \right\}
 \end{aligned}
 \tag{181} \text{ cont'd}$$

where,

$$\begin{aligned}
 \text{a)} \quad \bar{z}(\eta) &= \frac{1}{2} f'(\eta) - \frac{R(\eta)}{R(\infty)} \\
 \text{b)} \quad R(\eta) &= \int_0^\eta [f''(\alpha) \mathcal{L}(\alpha)] d\alpha \\
 \text{c)} \quad \mathcal{L}(\alpha) &= \int_0^\alpha Q(\alpha) d\alpha \\
 \text{d)} \quad Q(\eta) &= \left\{ \frac{4[1 - c_2 f'(\eta)]^{1-m^*}}{f''(\eta)} \right\} \prod_{j=1}^{m^*} \left[ K_{j, \text{II}} + \frac{1}{2} \Delta_j f'(\eta) \right] \cdot \\
 &\quad \exp \left[ \frac{-\beta_1}{1 - c_2 f'(\eta)} \right]
 \end{aligned}
 \tag{182}$$

D. Detailed Solution for First-Order Kinetics With Pr = Sc = 1:

In the case of first-order kinetics, the free stream which is at temperature  $T_{\text{I}}$ , cf. figure 17a, will consist of a cold mixture of an exothermically decomposable fuel\* denoted by the subscript f, and an

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\* See footnote on page 82.

inert gas, denoted by the subscript d. Since the mean flow velocity at the surface of the plate vanishes, the fluid is relatively stagnant right near the plate. Fuel molecules which move into the immediate vicinity of the plate may thus be expected to stay near the hot plate for a period of time sufficient to insure decomposition to the product specie. The concentration of fuel will thus be assumed to vanish at the wall\*. The boundary conditions on the specie weight fraction are thus as follows:

At the cold boundary,  $\eta = +\infty$       At the hot boundary,  $\eta = 0$

$$\left. \begin{array}{ll} K_{f_I} = 1 - \epsilon & K_{f_{II}} = 0 \\ K_{d_I} = \epsilon & K_{d_{II}} = \epsilon \\ K_{p_I} = 0 & K_{p_{II}} = 1 - \epsilon \end{array} \right\} \quad (183)$$

In the above equation,  $\epsilon$  denotes the weight fraction of inert diluent present in the combustible stream. From equations 67b and 183:

$$\left. \begin{array}{l} \Delta_f = 1 - \epsilon \quad ; \quad \Delta_d = 0 \quad ; \quad \Delta_p = -(1 - \epsilon) \end{array} \right\} \quad (184)$$

Equation 182d assumes a particularly simple form in the case of a first-order reaction, for in this case  $m^* - 1 = 0$ . Noting that there is but one term in the product function of equation 182d, namely the term for  $j = f$ , the following expressions are obtained.

\* The comments on pages 108 - 110 with regard to the fact that this is but one of two reasonable a priori assumptions apply. The case where the concentration gradients vanish at the wall should also be carried out for comparison.



$$a) \quad Q(\eta) = (1-\epsilon) \bar{Q}(\eta)$$

where,

$$b) \quad \bar{Q}(\eta) = \frac{2f'(\eta)}{f''(\eta)} \exp\left[\frac{-\beta_1}{1 - c_2 f'(\eta)}\right]$$

(185)

The appropriate expressions for the first-approximation to the temperature, specie concentrations, mixture density, and characteristic stay time are obtained upon substituting equations 183-185 into equations 181 and 182:

$$a) \quad z^{(1)}(\eta, \lambda) = \frac{1}{2} f'(\eta) - \lambda \bar{z}(\eta)$$

$$b) \quad K_f^{(1)}(\eta, \lambda) = \left(\frac{1-\epsilon}{2}\right) f'(\eta) - \frac{\lambda}{c_1} \bar{z}(\eta)$$

$$c) \quad K_p^{(1)}(\eta, \lambda) = \left(\frac{1-\epsilon}{2}\right) [2 - f'(\eta)] + \frac{\lambda}{c_1} \bar{z}(\eta)$$

(186)

$$d) \quad K_d = \epsilon$$

$$e) \quad \rho^{(1)}(\eta, \lambda) = \frac{\rho M}{R T^{(1)}(\eta, \lambda)} \quad ; \quad T^{(1)}(\eta, \lambda) = T_{II} - (T_{II} - T_I) z^{(1)}(\eta, \lambda)$$

$$f) \quad (1-\epsilon) t^* = [b c_1 \bar{R}(\infty)]^{-1}$$

where:

$$\begin{aligned}
 \text{a)} \quad \bar{Z}(\eta) &= \frac{1}{2} f'(\eta) - \frac{\bar{R}(\eta)}{\bar{R}(\infty)} \\
 \text{b)} \quad \bar{R}(\eta) &\equiv \frac{R(\eta)}{1-\epsilon} = \int_0^\eta f''(\alpha) \bar{Z}(\alpha) d\alpha \\
 \text{c)} \quad \bar{Z}(\eta) &\equiv \frac{Z(\eta)}{1-\epsilon} = \int_0^\eta \bar{Q}(\alpha) d\alpha \\
 \text{d)} \quad \bar{Q}(\alpha) &= \frac{2f'(\alpha)}{f''(\alpha)} \exp\left[\frac{-\beta_1}{1-\epsilon_1 f'(\eta)}\right]
 \end{aligned}
 \tag{187}$$

From equations 186b, 186c, 187a, 187b, and 187c and the fact that  $f''(0) = 1.328$ , it follows that:

$$\left. \frac{\partial K_f^{(1)}}{\partial \eta} \right|_{\eta=0} = 0.664 \left[ 1 - \epsilon - \frac{\lambda}{c_1} \right]$$

$$\left. \frac{\partial K_p^{(1)}}{\partial \eta} \right|_{\eta=0} = -0.664 \left[ 1 - \epsilon - \frac{\lambda}{c_1} \right]$$

The net flux of fuel is to the wall and the net flux of product specie is from the wall when,

$$\lambda < [c_1(1-\epsilon)]$$

and is vice versa when:

$$\mathcal{N} > [C_1(1-\epsilon)]$$

Since  $C_1 > 1_+$ , the first condition which is physically reasonable holds for  $\mathcal{N} < 1_+$  and the second conditions which is unacceptable (since an unopposed reaction has been assumed) holds only for  $\mathcal{N} > 1_+$  in which case the present analysis is admittedly invalid due to the breakdown of the classic boundary layer assumptions. The specification of the concentrations along the wall thus yields reasonable results in the case of first-order kinetics. The integral,

$$\bar{\varphi}(\eta) = \int_0^\delta \left\{ \frac{2f'(\alpha)}{f''(\alpha)} \exp\left[ \frac{-\beta_1}{1-C_2 f'(\alpha)} \right] \right\} d\alpha \quad (188)$$

cannot be evaluated except by numerical methods. By a simple approximation, however, equation 188 can be reduced to an integrable form. The exponential term is the dominant term in the integrand; the term  $2f'(\alpha)/f''(\alpha)$  is relatively a very slowly varying function of the variable of integration,  $\alpha$ . It will obviously be better to approximate the slowly varying function than to tamper with the dominant exponential term. Furthermore, since the integrand peaks for a small value of  $\alpha$  and then rapidly drops off to negligible values, the approximation for the slowly varying function must be satisfactory only for small values of  $\alpha$ . The simplest acceptable approximation which will reduce equation 188 to an integrable form is utilized.

$$f''(\alpha) = 1.322 \quad (\text{valid for } \alpha \text{ small}) \quad (189)$$

The constant was determined by the method of weighted least squares.

A comparison between the approximation and the actual function is presented in figure 19. The integrand of equation 188 has significant value only over the range of  $\alpha$  for which the approximation is satisfactory. From equations 188 and 189:

$$\bar{f}_2(x) \doteq 1.513 \int_0^x \left\{ f'(\alpha) \exp\left[ \frac{-\beta_1}{1 - C_2 f'(\alpha)} \right] \right\} d\alpha \quad (190)$$

A comparison of the integrands of equations 188 and 190 is presented in figure 20 for typical values of  $\beta_1$  and  $C_2$ ; the agreement is entirely satisfactory. The variations of  $\beta_1$  and  $C_2$  with the appropriate parameters (cf. equation 59) are presented in figures 21 and 22 respectively.

Equation 190 can be simplified by introduction of the following variable of integration:

$$\psi = \frac{+\beta_1}{1 - C_2 f'(\alpha)} \quad (191)$$

From equations 189-191:

$$\text{a) } \bar{f}_2(x) = 1.145 \left( \frac{\beta_1}{C_2} \right) \int_{\beta_1}^{\beta_2(x)} \left\{ \frac{1}{\psi^2} - \frac{\beta_1}{\psi^3} \right\} e^{-\psi} d\psi \quad (192)$$

where,

$$\text{b) } \beta_2(x) = \frac{+\beta_1}{1 - C_2 f'(\alpha)}$$

Because of the repeated appearance of sums of integrals of the type of equation 192a, it will be convenient to define:

$$\mathcal{Q}_{l,k}(x) = \sum_{n=l}^k \left\{ d_n \int_{\beta_1}^{\beta_2(x)} \frac{e^{-x}}{x^n} dx \right\} \quad (193)$$

An evaluation of  $\mathcal{Q}_{l,k}(x)$  in terms of  $l, k, \beta_1, \beta_2(x)$  and the coefficients  $d_n$  is presented in Appendix C. From equations 192 and 193:

$$\bar{\mathcal{Q}}(x) = \left[ \frac{1.145 \beta_1}{c_2^2} \right] \mathcal{Q}_{2,3}(x) \quad (194)$$

$$\text{with: } \begin{cases} d_2 = 1 \\ d_3 = -\beta_1 \end{cases}$$

From equation C. 19:

$$\mathcal{Q}_{2,3}(x) = e^{-\beta_2(x)} \sum_{N=2}^{1+|\beta_2|} \frac{\rho_N}{[\beta_2(x)]^N} - e^{-\beta_1} \sum_{N=2}^{1+|\beta_1|} \frac{\rho_N}{\beta_1^N} \quad (195)$$

From equations 194, C. 16, and C. 17:

$$\rho_N = \begin{cases} -1 & N = 2 \\ \left[ \frac{(-1)^{N-1} (N-1)!}{2} \right] (\beta_1 + 2) & N \geq 3 \end{cases} \quad (196)$$

Substituting equation 195 into equation 194 and utilizing equation 192b:

$$\bar{\mathcal{Q}}(x) = \left[ \frac{1.145 \beta_1 e^{-\beta_1}}{c_2^2} \right] \left\{ \exp[-c_2 f'(x) \beta_2(x)] \cdot \sum_{N=2}^{1+|\beta_2|} \frac{\rho_N}{[\beta_2(x)]^N} - \sum_{N=2}^{1+|\beta_1|} \frac{\rho_N}{\beta_1^N} \right\} \quad (197)$$

Now define the quantities:

$$\begin{aligned}
 \text{a)} \quad I_N(\eta, \beta_1, c_2) &= \int_0^\eta \left\{ f''(\eta) [\beta_2(\eta)]^{-N} \exp[-c_2 f'(\eta) \beta_2(\eta)] \right\} d\eta \\
 \text{b)} \quad H(\beta) &= -\beta_1^3 \sum_{N=2}^{1+|\beta_1|} (\beta_N / \beta_1^N) \\
 \text{c)} \quad A(c_2, \beta_1) &= \frac{1.145 e^{-\beta_1}}{\beta_1^2 c_2^3}
 \end{aligned}
 \tag{198}$$

Substituting equations 197 and 198 into equation 187b and carrying out the integration of the second term, noting from Table I that  $f'(0) = 0$  :

$$\bar{R}(\eta) = A \beta_1^3 c_2 \left\{ \sum_{N=2}^{1+|\beta_1|} [\beta_N I_N(\eta)] + \frac{H(\beta)}{\beta_1^3} f'(\eta) \right\}
 \tag{199}$$

Equation 198a can be placed in a more tractable form by introducing a new variable of integration:

$$z = \beta_2(\eta)
 \tag{200}$$

Equation 198a can then be written in the form:

$$I_N(\eta) = \frac{\beta_1 e^{\beta_1}}{c_2} \int_{\beta_1}^{\beta_2(\eta)} \left( \frac{e^{-z}}{z^{N+2}} \right) dz
 \tag{201}$$

If the following definition is now introduced (cf. equation 146),

$$D_n = \rho_{n-2} = \begin{cases} -1 & ; N = 4 \\ \left[ \frac{(-1)^{n-1} (n-3)! (\beta_1 + 2)}{2} \right] & ; N > 4 \end{cases} \quad (202)$$

then, from equations 201 and 202:

$$\sum_{N=2}^{1+|A_1|} [\rho_N I_N(\eta)] = \frac{\beta_1 e^{\beta_1}}{c_2} \sum_{n=4}^{3+|A_1|} \left\{ D_n \left( \frac{\beta_2(\eta)}{\beta_1} \right) \frac{e^{-z}}{z^n} dz \right\} \quad (203)$$

From equations C.1, C.19, C.17, and 203:

$$\sum_{N=2}^{1+|A_1|} [\rho_N I_N(\eta)] = \frac{\beta_1}{c_2} \left\{ \exp[-c_2 f'(\eta) \beta_2(\eta)] \cdot \sum_{N=4}^{1+|A_1|} \frac{\lambda_N}{[\beta_2(\eta)]^N} - \sum_{N=4}^{1+|A_1|} \left( \frac{\lambda_N}{\beta_1^N} \right) \right\} \quad (204)$$

where,

$$a) \quad \lambda_N = (-1)^{N-1} (N-1)! \rho_{4,N} \quad (205)$$

$$b) \quad \rho_{4,N} = \sum_{n=4}^N \frac{(-1)^n D_n}{(n-1)!}$$

Substituting equation 202 into equation 205b:

$$\begin{aligned}
 q_{4,4} &= -\frac{1}{6} \\
 q_{4,N} &= -\left[ \frac{1}{6} + \sum_{n=5}^N \left( \frac{\beta_1 + 2}{2} \right) \frac{(n-3)!}{(n-2)!} \right] \\
 &= -\left[ \frac{1}{6} + \left( \frac{\beta_1 + 2}{2} \right) \sum_{n=5}^N \frac{1}{(n-1)(n-2)} \right] \\
 &= -\left[ \frac{1}{6} + \left( \frac{\beta_1 + 2}{6} \right) \left( \frac{N-4}{N-1} \right) \right]
 \end{aligned}
 \quad \left. \vphantom{\begin{aligned} q_{4,4} \\ q_{4,N} \\ \\ q_{4,N} \end{aligned}} \right] \quad N > 4$$

Thus,

$$q_{4,N} = -\frac{1}{6(N-1)} [3(N-3) + \beta_1(N-4)] \quad ; \quad N > 4 \quad (206)$$

Substituting equation 206 into equation 205a:

$$\lambda_N = \left[ \frac{(-1)^N (N-2)!}{6} \right] [3(N-3) + (N-4)\beta_1] \quad ; \quad N > 4 \quad (207)$$

Now define,

$$\begin{aligned}
 \text{a) } L_1(\beta_1) &= \beta_1^4 \sum_{N=4}^{1+|\beta_1|} \left( \lambda_N / \beta_1^N \right) \\
 \text{b) } L_2(\eta, \beta_1, c_2) &= \beta_1^4 \exp[-c_2 f'(\eta) \beta_2(\eta)] \cdot \\
 &\quad \sum_{N=4}^{1+|\beta_2|} \left\{ \lambda_N / [\beta_2(\eta)]^N \right\}
 \end{aligned}
 \quad (208)$$

Substituting equation 208 into equation 204:



$$\sum_{N=2}^{1+|\beta_2|} [\rho_N I_N(\eta)] = \frac{1}{c_2 \beta_2^3} [L_2(\eta, \beta_1, c_2) - L_1(\beta_1)] \quad (209)$$

Now, from equations 199 and 209:

$$\bar{R}(\eta) = A(\beta_1, c_2) [L_2(\eta, \beta_1, c_2) - L_1(\beta_1) + c_2 f'(\eta) H(\beta_1)] \quad (210)$$

Simplified expressions for  $L_1(\beta_1)$ ,  $L_2(\eta, \beta_1, c_2)$ , and  $H(\beta_1)$  will now be obtained. From equations 198b and 196:

$$H(\beta_1) = \beta_1 + \sum_{N=3}^{1+|\beta_1|} \left[ \frac{(-1)^{N-1} (N-1)! (\beta_1+2)}{2 \beta_1^{N-2}} \right]$$

This expression simplifies to the following form:

$$H(\beta_1) = \sum_{N=0}^{|\beta_1|-3} \left[ \frac{(-1)^N (N+1)(N+2)!}{2 \beta_1^N} \right] \quad (211)$$

Substitution of equation 207 into equation 208a and simplification yields,

$$L_1(\beta_1) = \sum_{N=1}^{|\beta_1|-4} \left[ \frac{(-1)^{N+1} N(N+1)(N+2)!}{6 \beta_1^N} \right] \quad (212)$$

From equations 207 and 208b:

$$\exp[-c_2 f'(\eta) \beta_2(\eta)] L_2(\eta) = \beta_1^4 \sum_{N=4}^{1+|\beta_2|} \left[ \frac{(-1)^N (N-2)!}{6 \{\beta_2(\eta)\}^N} \right] \cdot [3(N-3) + (N-4)\beta_1] \quad (213)$$

The following definitions are now introduced:

$$\begin{aligned}
 \text{a)} \quad \Phi_N(\eta, \beta_1, c_2) &= \left\{ [1 - c_2 f'(\eta)]^{N+4} [(N+3)c_2 f'(\eta) - N] \cdot \right. \\
 &\quad \left. \exp \left[ \frac{-\beta_1 c_2 f'(\eta)}{1 - c_2 f'(\eta)} \right] \right\} \\
 \text{b)} \quad J_N(\beta_1) &= \left[ \frac{(-1)^N (N+1)(N+2)!}{6 \beta_1^N} \right]
 \end{aligned} \tag{214}$$

The following expressions are obtained by substitution of equation 214 into equations 211, 212, and 213:

$$\begin{aligned}
 \text{a)} \quad H(\beta_1) &= 3 \sum_{N=0}^{12} J_N(\beta_1) \\
 \text{b)} \quad L_1(\beta_1) &= - \sum_{N=0}^{12} [N J_N(\beta_1)] \\
 \text{c)} \quad L_2(\eta, \beta_1, c_2) &= \sum_{N=0}^{12} [J_N(\beta_1) \Phi_N(\eta, \beta_1, c_2)]
 \end{aligned} \tag{215}$$

The upper limits of all three sums have rather arbitrarily been set equal to 12; numerical calculations indicate that this convenience does not incur significant error. Plots of the functions  $H(\beta_1)$  and  $L_1(\beta_1)$  are presented in figures 23 and 24 respectively. Fortunately the functions are smooth and may be accurately obtained from large scale plots on graph paper without continual resort to the rather lengthy

numerical evaluation of equations 215a and 215b.

If equation 215 is now substituted into equation 210, the following expression is finally obtained for the integral  $\bar{R}(\eta)$  :

$$\bar{R}(\eta) = A(\beta_1, c_2) \sum_{N=0}^{\infty} \left\{ J_N(\beta_1) \left[ 3c_2 f'(\eta) + N + \Phi_N(\eta, \beta_1, c_2) \right] \right\} \quad (216)$$

The cold boundary condition (cf. footnote page 82 ) requires that the exponential term in equation 214a be set equal to zero when  $T \leq T_x$  or, equivalently, when  $\eta = \infty$  ; thus,

$$\Phi_N(\eta = \infty, \beta_1, c_2) = 0 \quad (217)$$

Utilizing equations 215a, 215b, 216, and 217, the following expression which will be employed in calculating characteristic stay times is obtained:

$$\bar{R}(\infty) = A(\beta_1, c_2) \left[ 2c_2 H(\beta_1) - L_1(\beta_1) \right] \quad (218)$$

The relation  $f'(\infty) = 2$ , cf. Table I, has been utilized in obtaining equation 218. The following useful parametric representation of the characteristic stay time is obtained from equations 59, 186f, 198c, and 218:

$$\begin{aligned}
 \text{a)} \quad & \log_{10} \left[ (1-\epsilon) b t^* \left( T_f/T_x - 1 \right) \right] \\
 & = 0.4343 \left\{ \beta_1 + \log_{10} \left[ \frac{(a-1)^4}{a^3} \frac{0.1092 \beta_1^2}{\frac{a-1}{a} H(\beta_1) - L_1(\beta_1)} \right] \right\}
 \end{aligned} \tag{219}$$

with,

$$\text{b)} \quad a \equiv T_{II}/T_I$$

The logarithmic term on the right hand side is small in comparison to the  $\beta_1$  term; the left hand side is thus essentially a linear function of  $\beta_1$ , cf. figure 25. The parametric plot in figure 25 is useful in that none of the parameters of the system have been specified. For given values of the activation energy and of the free stream and plate temperatures,  $\beta_1$  can be obtained from figure 21 and the parameter  $T_{II}/T_I$  evaluated. Figure 25 will then yield the value of any one of the quantities  $t^*$ ,  $\epsilon$ ,  $b$ , or  $T_f$  when the other three are specified. The variation of the characteristic stay time with the plate and free stream temperatures for fixed values of  $T_f$ ,  $E$ , and  $b$ , corresponding to the decomposition of azomethane, is presented in figure 26. As indicated, the characteristic stay time (or, equivalently, the characteristic attachment distance) rapidly exceeds practical values as the plate temperature decreases. Note that figure 26 would be very similar to figure 7, for the mixing region case, if plotted on semi-log paper.

The function  $\bar{R}(\eta)$ , as calculated from equations 198c, 214, and 216 is presented in figure 27; the values of the physical parameters

correspond to the decomposition of azomethane. The values of  $f'(\eta)$  are taken from Table I. Using the previously calculated values of  $\bar{R}(\eta)$  and  $\bar{R}(\infty)$ , the temperature and specie concentration profiles during the early stages of a first-order reaction in a laminar boundary layer are calculated using equations 186 and 187a. The temperature profiles are presented in figure 28; the development of a temperature bulge at the wall is clearly indicated. The specie concentration profiles are presented in figure 29; note the similarity with figure 6, for the mixing region case.

E. Detailed Solution for Second-Order Kinetics with  $Pr = Sc = 1$ :

In the case of second-order kinetics, the free stream which is at temperature  $T_I$ , cf. figure 17a, will consist of a cold mixture of fuel, denoted by the subscript f, of oxidizer, denoted by the subscript o, and of inert diluent, denoted by the subscript d. At the cold boundary,  $\eta = \infty$ , the specie weight fractions have the following values:

At the cold boundary,  $\eta = \infty$  :

$$\left. \begin{aligned} K_{f_I} &= (1-\epsilon) \left( \frac{\phi_o}{1+\phi_o} \right) & K_{o_I} &= \left( \frac{1-\epsilon}{1+\phi_o} \right) \\ K_{p_I} &= 0 & K_{d_I} &= \epsilon \end{aligned} \right\} \quad (220)$$

In the above expressions,  $\phi_o$  and  $\epsilon$  denote the free stream equivalence ratio and weight fraction of inert diluent respectively.

Even for the case where the concentrations are to be specified

along the plate surface<sup>\*</sup>, the boundary conditions are not a priori evident. One reasonable a priori assumption is that the specie concentrations at the hot surface are identical with those which would exist far downstream of a plane laminar flame front. There would thus be an excess of oxidizer at the wall if the free stream equivalence ratio were less than unity, and an excess of fuel at the wall if the free stream equivalence ratio were greater than unity. Only for the particular case of a free stream stoichiometric mixture would there be an absence of both fuel and oxidizer at the wall. The corresponding boundary conditions at the wall are as follows:

At the hot boundary,  $\eta = 0$  (assuming same conditions as far downstream of a laminar flame front):

$$\left. \begin{aligned}
 K_{F_H} &= \begin{cases} 0 & ; \phi_o \leq 1 \\ (1-\epsilon) \left( \frac{\phi_o - 1}{1 + \phi_o} \right) & ; \phi_o > 1 \end{cases} \\
 K_{O_H} &= \begin{cases} (1-\epsilon) \left( \frac{1 - \phi_o}{1 + \phi_o} \right) & ; \phi_o < 1 \\ 0 & ; \phi_o \geq 1 \end{cases} \\
 K_{P_H} &= \begin{cases} (1-\epsilon) \left( \frac{2\phi_o}{1 + \phi_o} \right) & ; \phi_o < 1 \\ (1-\epsilon) \frac{2}{1 + \phi_o} & ; \phi_o \geq 1 \end{cases}
 \end{aligned} \right\} ; K_{d_H} = \epsilon \quad (221)$$

An alternative specification of the specie weight fractions at

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\* The comments on pages 108 - 110 with regard to the fact that this is but one of two reasonable a priori assumptions apply. The case where the concentration gradients vanish at the wall should also be carried out for comparison.

the wall assumes that regardless of the free-stream equivalence ratio, neither fuel nor oxygen species successfully penetrate to the wall.

At the hot boundary,  $\eta = 0$  (assuming neither fuel nor oxidizer at the wall):

$$\left. \begin{aligned} K_{f_{\pi}} &= 0 & K_{o_{\pi}} &= 0 \\ K_{p_{\pi}} &= 1 - \epsilon & K_{d_{\pi}} &= \epsilon \end{aligned} \right\} (222)$$

The dependence of the characteristic stay time upon free stream equivalence ratio will be determined for each of the two assumptions of specie concentrations along the wall.

In the case of a second-order reaction,  $m^* = 2$ . Thus, from equations 67b, 182b, 182c, 182d, and 220:

$$\left. \begin{aligned} \text{a)} \quad Q(\eta) &= \frac{4 \left\{ K_{o_{\pi}} \left[ 1 - \frac{f'(\eta)}{2} \right] + \frac{f'(\eta)}{2} \left( \frac{1-\epsilon}{1+\phi_0} \right) \right\} \left\{ K_{f_{\pi}} \left[ 1 - \frac{f'(\eta)}{2} \right] + \frac{f'(\eta)}{2} \phi_0 \left( \frac{1-\epsilon}{1+\phi_0} \right) \right\}}{f''(\eta) [1 - c_2 f'(\eta)]} \\ &\quad \cdot \exp \left[ \frac{-\beta_1}{1 - c_2 f'(\eta)} \right] \\ \text{b)} \quad \mathcal{L}(\eta) &= \int_0^{\eta} Q(\alpha) d\alpha \\ \text{c)} \quad R(\eta) &= \int_0^{\eta} [f''(\eta) \mathcal{L}(\eta)] d\eta \end{aligned} \right\} (223)$$

From equation 181f:

$$\left( t_{\phi_0}^* / t_{\phi_0=1}^* \right) = \left\{ \frac{R(\infty) |_{\phi_0=1}}{R(\infty) |_{\phi_0}} \right\} \quad (224)$$

For the particular case  $\phi_0 = 1$ , equations 221 and 222 agree that

$$K_{f_{II}} = K_{o_{II}} = 0; \text{ thus, from equation 223:}$$

$$R(\infty) |_{\phi_0=1} = \frac{(1-\epsilon)^2}{4} \int_0^\infty \left\{ f''(\eta) \int_0^\eta \left[ \frac{\{f'(\alpha)\}^2}{1-c_2 f'(\alpha)} \right] \exp\left[ \frac{-\beta_1}{1-c_2 f'(\alpha)} \right] d\alpha \right\} d\eta \quad (225)$$

Assuming that the specie concentrations at the plate surface are correctly given by equation 222, it follows from equation 223 that:

$$R(\infty) |_{\phi_0} = \left( \frac{1-\epsilon}{1+\phi_0} \right)^2 \phi_0 \int_0^\infty \left\{ f''(\eta) \int_0^\eta \left[ \frac{\{f'(\alpha)\}^2}{1-c_2 f'(\alpha)} \right] \exp\left[ \frac{-\beta_1}{1-c_2 f'(\alpha)} \right] d\alpha \right\} d\eta \quad (226)$$

Thus, when equation 222 is valid:

$$\left( t_{\phi_0}^* / t_{\phi_0=1}^* \right) = \frac{(1+\phi_0)^2}{4\phi_0} \quad (227)$$

Note that equation 227 is identical with equation 125 for the mixing region case in which  $T_{II} = \text{constant}$ . The variation of the characteristic stay time with equivalence ratio, as given by equation 227, is presented in figure 30. This variation is substantially in agreement with unpublished experimental studies by the present author and by D. Turcotte.



If the boundary conditions at the wall are assumed to be given by equation 221, the integrands in equation 223 are not independent of  $\phi_0$ , as in the previous case, and the variation of the characteristic stay time with equivalence ratio, according to equation 224, must be determined by numerical integration. If equation 221 is substituted into equation 223a, and the integrals of equations 223b and 223c are evaluated numerically for various values of  $\phi_0$ , the results may be substituted into equation 224 to yield the variation of characteristic stay time with equivalence ratio. The results of such calculations are presented in figure 31. These results are in complete disagreement with available experimental evidence and with intuitive reasoning; one would expect the stay time to be at a minimum (and the blowoff velocity at a maximum) for an equivalence ratio near stoichiometric. Figure 30 agrees with this reasoning, and the available experimental evidence, while figure 31 is in complete contradiction. The obvious conclusion is that if the specification of the concentration, rather than the concentration gradient, along the wall is valid then the specification must be that of equation 222 and not that of equation 221. An explanation for the apparent validity of the boundary conditions as given by equation 222 is presented in the following paragraph.

In the region of initial chemical reaction, the local equivalence ratio is as follows; cf. equations 182d and 220:

$$\phi(\eta) = \frac{K_{F_x}^{(0)}(\eta)}{K_{O_2}^{(0)}(\eta)} = \left\{ \frac{K_{F_x} \left[ 1 - \frac{f(\eta)}{2} \right] + \phi_0 \left( \frac{1-\epsilon}{1+\phi_0} \right)}{K_{O_2} \left[ 1 - \frac{f(\eta)}{2} \right] + \left( \frac{1-\epsilon}{1+\phi_0} \right)} \right\} \quad (228)$$

If the wall conditions of equation 221 are substituted into equation 228, it is apparent that the local equivalence ratio near the wall, where the initial reaction will take place, may vary considerably from the free stream value of the equivalence ratio:

$$\phi(\eta) = \begin{cases} \phi_0 \left[ 1 + (1 - \phi_0) \left\{ 1 - \frac{1}{2} f'(\eta) \right\} \right]^{-1} & \phi_0 < 1 \\ \frac{(1 + \phi_0)^2}{4\phi_0} & \phi_0 = 1 \\ \phi_0 + (\phi_0 - 1) \left[ 1 - \frac{1}{2} f'(\eta) \right] & \phi_0 > 1 \end{cases} \quad (229)$$

Note, that except for the particular case  $\phi_0 = 1$ , the local equivalence ratio is less than the free stream value when the latter is less than unity and is greater than the free stream value when the latter is greater than unity. Thus the local fuel-oxidizer ratio is always further removed from the desirable stoichiometric ratio than is the free stream mixture.

If the wall conditions of equation 222 are substituted into equation 228, it is apparent that in the region of initial chemical reaction the local equivalence ratio is always equal to the free stream value. This is reasonable in view of the fact that in the region of initial chemical reaction nothing has occurred which would substantially change the free stream value of the equivalence ratio. It is thus concluded that the wall boundary conditions of equation 222 are potentially valid while those of equation 221 are definitely invalid. A complete vindication of the boundary conditions of equation 221 must await a

comparison with the results of an analysis in which the concentration gradients are set equal to zero at the wall. In the meantime, it can be accurately stated that none of the results of the present analysis, in which the concentrations are specified at the wall, are in essential conflict with reality.

The variation of the characteristic stay time with static pressure and with the extent of vitiation is the same as for the mixing region case, Part III. The static pressure dependence is given in equation 123 and in figure 9; the dependence upon vitiation is given by equations 124, 131, and 132 and is presented in figure 11. Temperature and concentration profiles can be determined using equations 181, 192, and 223. The profiles will be very similar to those for the case of first-order kinetics; cf. figures 28 and 29.

## VI. RÉSUMÉ AND CONCLUDING REMARKS

The analysis of Marble and Adamson<sup>(8)</sup> for combustion in a laminar mixing region has been substantially modified and extended. The modification consists of the elimination of the partial differential equations for the chemical specie concentrations by means of a similarity solution and the utilization of an iterative technique rather than the classic perturbation technique for the solution of the energy equation. The present analysis extends the approach of Marble and Adamson to the problem of second-order and third-order kinetics in the laminar mixing region of arbitrary velocity ratio and to combustion, according to first-order, second-order, or third-order kinetics, within the laminar boundary layer of a constant temperature flat plate. The extension of the similarity solution to problems in one-dimensional reacting flow systems is briefly discussed in Appendix E. The constant temperature restriction in the flat plate problem is removed in Appendix F, and the application of the similarity solution to the interesting problem of dissociation and recombination in the hypersonic laminar boundary layer is discussed in Appendix G.

The basic analysis which is generally applicable to boundary layer type flow systems with chemical reaction is developed in Part II. The general governing relations for flowing gaseous systems with chemical reaction are discussed; they are then simplified for the particular case of a one-step unopposed, "global" reaction occurring in a laminar boundary layer type region. The expressions for the transport properties and flux vectors are considerably simplified through the assumption of mechanically similar Maxwellian molecules.

The Howarth transformation is then utilized to reduce the governing relations to the corresponding constant density form. A similarity function relating the specie concentrations to the local temperature is found for the case of equal Prandtl and Schmidt numbers. The similarity function is shown to be equal to the dimensionless stream-wise velocity when the Prandtl and Schmidt numbers are both equal to unity. The governing relations are then transformed to the Blasius plane in which the velocity field has known solutions.

The particular case of combustion within a laminar mixing region whose velocity ratio is equal to unity is discussed in Part III. An exact analytic solution is obtained for the similarity function and an iterative technique is employed for the solution of the energy equation; a general solution for the N'th approximation is obtained. In the case of first-order kinetics, the results of the present analysis are found to be in satisfactory agreement with those of the Marble-Adamson analysis. Both premixed and diffusion flames are considered in the case of second-order kinetics; the results will be summarized shortly.

Combustion within a laminar mixing region with arbitrary velocity ratio is considered in Part IV. The solution of Görtler<sup>(58)</sup> for the velocity field is utilized. The similarity function and the dimensionless temperature are obtained in a manner analogous with the previous case. For a given cold stream velocity, it is determined that the characteristic stay time and attachment length decreases with decreasing hot stream velocity.

Combustion within the laminar boundary layer of a constant temperature flat plate is considered in Part V. As in the case of the mixing region, it is found that due to the consideration of a semi-infinite domain in which reaction can occur, a temperature bulge always develops. However, when the temperature of the flat plate (corresponding to the hot stream temperature in the mixing region case) falls below a critical value, the characteristic attachment length and stay time become so large that a flame would "blowoff" any reasonably sized apparatus.

The second-order reaction is of prime technological importance. The present analysis yields the following conclusions: (1) the blowoff velocity (which is inversely proportional to the characteristic stay time) is directly proportional to the static pressure, and (2) the blowoff velocity is also directly proportional to  $(1 - \epsilon)^2$  where  $\epsilon$  is the weight fraction of inert diluent present in the combustible mixture. The analysis also yields expressions for the dependence of blowoff velocity upon equivalence ratio. A careful check of the analysis reveals that these functional relations are independent of many of the restrictive assumptions of the present analysis. Since the mixing region is a reasonably good model for flame stabilization in the separated boundary layer behind a bluff body flame stabilizer, it might be expected that the present analysis would, in the case of second-order kinetics, be in qualitative agreement with experiment. In fact, surprisingly good quantitative agreement with available experimental data is obtained with regard to the dependence of stay time (or, equivalently of blowoff

velocity) upon static pressure, extent of vitiation and equivalence ratio. The application of the functional relations such as those of this analysis may reduce the amount of experimental data which must be obtained in developing turbojet afterburner combustors or other technologically important combustion devices. A successful coupling of quantitative experimental data with analytically derived functional correlations appears to be feasible.

The similarity solutions of the present analysis may readily be extended to other combustion problems of technological importance. Without modification, or with only slight modification, the following problems should prove to be amenable to treatment by the present analysis:

1. Flame stabilization within the laminar boundary layer of a finite flat plate; through extension of Appendix F.
2. Dissociation and recombination in the hypersonic laminar boundary layer of a flat plate; through extension of Appendix G in the case of constant wall temperature, and through the extension of Appendix G with modifications from Appendix F in the case of a wall with arbitrary temperature distribution.
3. The thermal quenching of a flame front obliquely penetrating the boundary layer of a cold wall; through modification of Part V; Appendix F should be utilized if the restriction of a constant wall temperature is not acceptable. The angle at which the flame front penetrates the boundary layer must be small if the classic boundary layer assumptions are

to be valid; cf. page 112.

4. The erosive burning of a solid propellant grain; requires modification of the equation of mass conservation, equation 2, for the presence of mass sources along the wall.
5. The axially symmetric diffusion flame; through extension of Section III D. 2 with modifications from Part IV.
6. Planar, cylindrical, or spherical, one-dimensional time dependent ignition problems; through extension of Appendix E.

In a rather broad sense, the present analysis reemphasizes the conclusion of Marble and Adamson: namely, that there exists a wide class of technologically important combustion problems which are accessible, at least with respect to disclosing the essential features, with present analytic techniques.



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## APPENDIX A

### SUMMARY OF ASSUMPTIONS

The assumptions basic to the present analysis are herein summarized for convenience. The numbers within parenthesis refer to the page on which the assumption under discussion was first introduced into the text. The motivation for introducing a given assumption is discussed where the assumption is introduced into the text.

1. Assumptions Fundamental to the Boltzmann Integro-Differential Equation .
  - a. The density is sufficiently low that the effect of collisions involving more than two molecules is negligible; only binary collisions are considered (4) .
  - b. The gas mixture behaves as a continuum; the mean free path of the gas molecules must thus be short compared with all of the macroscopic dimensions of the system (4) .
2. Assumptions Fundamental to the Navier-Stokes Equations .
  - a. The gradients in physical properties are small in the sense that they do not change appreciably in a distance of a mean free path (5) .
  - b. Classical mechanics, rather than quantum mechanics, is employed (6) .
  - c. The gas medium is isotropic (13) .
  - d. The normal and shear stresses are linear functions of the deformation velocities (13) .

e. The coefficient of bulk viscosity is small and may be set equal to zero (14) .

3. Assumptions with Respect to Molecular Properties .

- a. With respect to the interchange of angular momentum, the molecules act as smooth spheres; thus no interchange of angular momentum is possible (8) .
- b. Each component of the gas mixture obeys the thermodynamic equation of state of a perfect gas (9) .
- c. The gas mixture obeys Dalton's law (10) .
- d. The gas mixture consists of mechanically similar molecules (18); thus,
- 1) the molecular weights of all species are equal .
  - 2) the molecules of all species obey the same law of interaction at encounter .
- e. The molecules are Maxwellian (18).
- f. The Eucken correction for the thermal conductivity of polyatomic molecules is employed (19) .
- g. The components of the gas mixture are all calorically perfect (20).
- h. The specific heats of the various chemical species are equal (20).
- i. The reaction-rate laws of classical chemical kinetics are applicable (21) .
- j. Only one-step chemical reactions are considered (22) .



k. The backward reaction is negligible (22). This assumption is not employed in Appendix G.

. The law of mass action is utilized (23).

m. The specific reaction-rate coefficient is given by the Arrnehius law (23).

#### 4. Assumptions With Respect to the Flow System

a. No sources or sinks for mass are present in the flow system (7).

b. The transfer of energy by radiation is neglected (16).

c. All viscous regions and flame fronts are laminar (30).

d. No external forces act upon the gas molecules (30).

e. The flow field is a constant pressure flow field (31).

f. The ratio of thermal to kinetic energy is so high as to make the viscous dissipation function negligible (35). This assumption is not employed in Appendix G.

g. The classic Prandtl boundary layer assumptions are applicable (39): also refer to the discussions on pages 39-40, 68, and 112.

h. The boundary conditions are independent of the streamwise coordinate (48). This restriction is eliminated in Appendix F for the case of combustion within the laminar boundary layer of a flat plate.

#### 5. Assumptions Fundamental to Similarity Solutions

a. The assumption  $Pr = Sc$  (52) is fundamental to all of the analyses of the present paper.

- b. The assumption  $Pr = Sc = 1$  (57) is not fundamental to any of the analyses of the present paper; this assumption, however, greatly reduces the labor of the numerical calculations.

APPENDIX B

SOLUTION OF PERTINENT ORDINARY DIFFERENTIAL EQUATIONS

1. From equation 87 of the text,

$$\frac{d^2F}{d\eta^2} + 2Pr\eta \frac{dF}{d\eta} = 0$$

with,

$$F(\eta) = \begin{cases} 1 & ; \eta = +\infty \\ 0 & ; \eta = -\infty \end{cases}$$

(B. 1)

Define  $\epsilon = dF/d\eta$  , then

$$\frac{d\epsilon}{d\eta} + 2Pr\eta\epsilon = 0$$

(B. 2)

Equation B. 2 is a first-order, homogeneous, linear differential equation which has an integrating factor of  $\exp(Pr \eta^2)$  ; thus equation B. 2 may be expressed as,

$$\frac{d}{d\eta} [\epsilon \exp(Pr\eta^2)] = 0$$

Integration of the above equation and the replacement of  $\epsilon$  by its equivalent  $dF/d\eta$  , yields the following,

$$\frac{dF}{d\eta} = A \exp(-Pr\eta^2)$$

(B. 3)

where A is the constant of integration. If equation B. 3 is now integrated from  $-\infty$  to  $\eta$  and the second boundary condition of equation B.1 is applied, then

$$F(\eta) = A \int_{-\infty}^{\eta} \exp(-Pr \bar{x}^2) d\bar{x}$$

The variable of integration is now changed to  $\alpha = \bar{x}\sqrt{Pr}$  and the error function (a tabulated function, cf., reference 71) which is defined as

$$\operatorname{erf} x \equiv \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt \quad (\text{B. 4})$$

is introduced. Thus,

$$F(\eta) = \frac{A}{2} \sqrt{\frac{\pi}{Pr}} \left[ \operatorname{erf}(\eta\sqrt{Pr}) - \operatorname{erf}(-\infty) \right] \quad (\text{B. 5})$$

The constant of integration, A, is now obtained upon evaluating equation B.5 at  $+\infty$ ; the first boundary condition of equation B.1 is applied and the relation  $\operatorname{erf}(\infty) = -\operatorname{erf}(-\infty) = 1$  is utilized.

$$\frac{A}{2} \sqrt{\frac{\pi}{Pr}} = \frac{1}{2} \quad (\text{B. 6})$$

The final solution to equation B.1 is obtained upon substitution of equation B.6 into equation B.5.

$$F(\eta) = \frac{1}{2} \left[ 1 + \operatorname{erf}(\eta\sqrt{Pr}) \right] \quad (\text{B. 7})$$

The above solution appears as equation 88 in the main body of the text.

2. From equation 92 of the text,

$$\frac{d^2 z^{(N)}}{d\eta^2} + 2Pr\eta \frac{dz^{(N)}}{d\eta} = PrX(x) e^{-Pr\eta^2} Q^{(N-1)}(\eta, x)$$

with,

$$z^{(N)}(\eta, x) = \begin{cases} 1 & ; \eta = +\infty \\ 0 & ; \eta = -\infty \end{cases}$$

(B. 8)

if  $x$  is temporarily treated as a constant, then equation B.8 can be written as an ordinary differential equation for any fixed value of  $x$ .

Thus,

$$\frac{d^2 z^{(N)}}{d\eta^2} + 2Pr\eta \frac{dz^{(N)}}{d\eta} = PrX(x) e^{-Pr\eta^2} Q^{(N-1)}(\eta, x)$$

with,

$$z^{(N)}(\eta, x) = \begin{cases} 1 & ; \eta = +\infty \\ 0 & ; \eta = -\infty \end{cases}$$

(B. 9)

Now define  $\epsilon = dz^{(N)}/d\eta$ , then the above equation may be rewritten as

$$\frac{d\epsilon}{d\eta} + 2Pr\eta\epsilon = PrX(x) e^{-Pr\eta^2} Q^{(N-1)}(\eta, x)$$

(B. 10)

Equation B. 10 is a first-order, nonhomogeneous, linear differential equation which has an integrating factor of  $\exp(Pr\eta^2)$ ; thus equation B. 10 may be expressed as,

$$\frac{d}{d\eta} [\epsilon \exp(P_r \eta^2)] = P_r \mathbb{I}(x) Q^{(N-1)}(\eta, x)$$

The above equation is now integrated at constant  $x$  from  $\eta = 0$  to  $\eta$  and  $\epsilon$  is then replaced by its equivalent  $d_z^{(N)}/d\eta$ . Thus,

$$\left. \frac{d_z^{(N)}}{d\eta} = e^{-P_r \eta^2} \left\{ \frac{d_z^{(N)}}{d\eta} \Big|_{\eta=0} + P_r \mathbb{I}(x) \int_0^\eta Q^{(N-1)}(\bar{\alpha}, x) d\bar{\alpha} \right\} \right] \quad (B. 11)$$

Equation B. 11 is now integrated from  $-\infty$  to  $\eta$  at constant  $x$  and the second boundary condition of equation B. 9 is applied. The following result is obtained.

$$\left. \begin{aligned} z^{(N)}(\eta, x) &= \frac{d_z^{(N)}}{d\eta} \Big|_{\eta=0} \int_{-\infty}^\eta e^{-P_r \bar{\alpha}^2} d\bar{\alpha} \\ &+ P_r \mathbb{I}(x) \int_{-\infty}^\eta \left\{ e^{-P_r \bar{\delta}^2} \int_0^{\bar{\delta}} Q^{(N-1)}(\bar{\alpha}, x) d\bar{\alpha} \right\} d\bar{\delta} \end{aligned} \right] \quad (B. 12)$$

The variables of integration are now changed to  $\alpha = \bar{\alpha} \sqrt{P_r}$  and  $\delta = \bar{\delta} \sqrt{P_r}$  and the error function, defined in equation B. 4, is introduced. Then,

$$\left. \begin{aligned} z^{(N)}(\eta, x) &= \frac{1}{2} \sqrt{\frac{\pi}{P_r}} \frac{d_z^{(N)}}{d\eta} \Big|_{\eta=0} [1 + \text{erf}(\eta \sqrt{P_r})] \\ &+ \mathbb{I}(x) \int_{-\infty}^{\eta \sqrt{P_r}} \left\{ e^{-\delta^2} \int_0^\delta Q^{(N-1)}\left(\frac{\alpha}{\sqrt{P_r}}, x\right) d\alpha \right\} d\delta \end{aligned} \right] \quad (B. 13)$$

Equation B. 7 is now substituted in equation B. 13 and two new definitions are introduced. Thus,

$$\mathcal{Z}^{(N)}(\eta, x) = \sqrt{\frac{\pi}{Pr}} \left. \frac{d\mathcal{Z}^{(N)}}{d\eta} \right|_{\eta=0} F(\eta) + \Sigma(x) R^{(N-1)}(\eta, x) \quad (B. 14)$$

where:

$$a) \quad R^{(N-1)}(\eta, x) = \int_{-\infty}^{\eta\sqrt{Pr}} e^{-\eta^2} \mathcal{Z}^{(N-1)}(\eta, x) d\eta$$

(B. 15)

and

$$b) \quad \mathcal{Z}^{(N-1)}(\eta, x) = \int_0^{\eta\sqrt{Pr}} Q^{(N-1)}\left(\frac{\alpha}{\sqrt{Pr}}, x\right) d\alpha$$

Equation B. 14 is now evaluated at  $\eta = +\infty$ , using the first boundary condition of equations B. 1 and B. 9, and the constant coefficient of  $F(\eta)$  is determined.

$$\sqrt{\frac{\pi}{Pr}} \left. \frac{d\mathcal{Z}^{(N)}}{d\eta} \right|_{\eta=0} = [1 - \Sigma(x) R^{(N-1)}(\infty, x)] \quad (B. 16)$$

The final solution to equation B. 9, which is also the solution to equation B. 8, is obtained upon the substitution of equation B. 16 into equation B. 14.

$$a) \quad z^{(N)}(\eta, x) = F(\eta) - \Sigma(x) z^{(N-1)}(\eta, x)$$

where,

$$b) \quad z^{(N-1)}(\eta, x) = [F(\eta) R^{(N-1)}(\infty, x) - R^{(N-1)}(\eta, x)]$$

(B.17)

The above expressions appear in equations 93 and 94 in the main body of the text.

An expression for the first derivative with respect to  $\eta$  of  $z^{(N)}(\eta, x)$  is also required in the main body of the text. From equations B.11, B.15, and B.16 it follows that,

$$\frac{\partial z^{(N)}}{\partial \eta} = \left\{ \sqrt{\frac{Pr}{\pi}} \left[ 1 - \Sigma(x) R^{(N-1)}(\infty, x) \right] + \sqrt{Pr} \Sigma(x) z^{(N-1)}(\eta, x) \right\} e^{-Pr\eta^2}$$

(B.18)

The above expression appears as equation 97 in the main body of the text.

3. From equations 151 and 162 of the text,

$$a) \quad \frac{d^2 F}{d\eta^2} + Pr f(\eta) \frac{dF}{d\eta} = 0$$

with,

$$b) \quad F(\eta) = \begin{cases} 1 & ; \quad \eta = +\infty \\ 0 & ; \quad \eta = \eta_I \end{cases}$$

(B.19)



The hot boundary in the case of the mixing region is  $\eta_{\text{H}} = -\infty$  ;  
 in the case of the boundary layer, the hot boundary is given by  $\eta_{\text{H}} = 0$ .  
 Now define  $\epsilon = dF/d\eta$  ; then from equation B. 19a,

$$\left. \frac{d\epsilon}{d\eta} + \text{Pr} f(\eta)\epsilon = 0 \right] \quad (\text{B. 20})$$

Equation B. 20 is a first-order, homogeneous, linear differential equation which has an integrating factor,  $\mathcal{Q}(\eta)$ , given by

$$\left. \mathcal{Q}(\eta) = a \exp \int_0^\eta \text{Pr} f(\alpha) d\alpha \right] \quad (\text{B. 21})$$

where  $a$  is any non-zero constant. The integrating factor may be expressed in a more convenient form through the use of equation 143b of the text (or, equivalently, through the use of equation 160a of the text).

$$\left. \begin{aligned} \int_0^\eta \text{Pr} f(\alpha) d\alpha &= -\text{Pr} \int_0^\eta \frac{f'''(\alpha)}{f''(\alpha)} d\alpha \\ &= -\text{Pr} \int_{f''(0)}^{f''(\eta)} \frac{df''}{f''} \\ &= \ln_e \left[ \frac{f''(0)}{f''(\eta)} \right]^{\text{Pr}} \end{aligned} \right] \quad (\text{B. 22})$$

Substituting equation B. 22 into equation B. 21 and setting  $a = [f''(0)]^{-\text{Pr}}$ ,

$$\left. \mathcal{Q}(\eta) = [f''(\eta)]^{-\text{Pr}} \right] \quad (\text{B. 23})$$

Utilization of equation B. 23 as the integrating factor of equation B. 20 yields the following differential equation:

$$\frac{d}{d\eta} \left[ \epsilon \{ f''(\eta) \}^{-Pr} \right] = 0$$

The above differential equation is now integrated and  $\epsilon$  is then replaced by its equivalent,  $dF/d\eta$  ; then

$$\frac{dF}{d\eta} = A [f''(\eta)]^{Pr} \tag{B.24}$$

where A is the constant of integration. If the above equation is now integrated from  $\eta_{\infty}$  to  $\eta$  and the second boundary condition of equation B.19b is applied, then

$$F(\eta) = A \int_{\eta_{\infty}}^{\eta} [f''(\alpha)]^{Pr} d\alpha \tag{B.25}$$

The first boundary condition of equation B.19b is now applied and the constant of integration is then determined from equation B.25.

$$A = \left[ \int_{\eta_{\infty}}^{\infty} \{ f''(\alpha) \}^{Pr} d\alpha \right]^{-1} \tag{B.26}$$

The solution to equation B.19 is now obtained upon substituting equation B.26 into equation B.25. Particular solutions for the mixing region case and for the boundary layer case are presented in the following equation.

Mixing region case,  $\eta_{II} = -\infty$  :

$$a) \quad F(\eta) = \frac{\int_{-\infty}^{\eta} [f''(\alpha)]^{Pr} d\alpha}{\int_{-\infty}^{\infty} [f''(\alpha)]^{Pr} d\alpha}$$

Boundary layer case,  $\eta_{II} = 0$  :

$$b) \quad F(\eta) = \frac{\int_0^{\eta} [f''(\alpha)]^{Pr} d\alpha}{\int_0^{\infty} [f''(\alpha)]^{Pr} d\alpha} \doteq \left\{ \frac{0.664 Pr^{1/3}}{(1.328)^{Pr}} \right\} \int_0^{\eta} [f''(\alpha)]^{Pr} d\alpha \quad (B. 27)$$

Equations B. 27a and B. 27b appear as equations 152 and 163 respectively in the main body of the text.

The last expression in equation B. 27b is based upon the following approximation by E. Pohlhausen<sup>(72)</sup>,

$$[f''(0)]^{-Pr} \int_0^{\infty} [f''(\alpha)]^{Pr} d\alpha \doteq [0.664 Pr^{1/3}]^{-1} \quad (B. 28)$$

and the tabulated value,  $f''(0) = 1.328$ , which was obtained from Table I of the present paper. A table comparing the Pohlhausen approximation with numerical evaluations of the integral is presented by Goldstein<sup>(73)</sup>; the agreement is excellent. Note that the Pohlhausen approximation is applicable only to the boundary layer case, not to the mixing region case.

4. From equations 146a and 167 of the text,

$$a) \quad \frac{\partial^2 z^{(N)}}{\partial \eta^2} + Pr f(\eta) \frac{\partial z^{(N)}}{\partial \eta} = \Sigma(x) Q^{(N-1)}(\eta, x) [f''(\eta)]^{Pr}$$

with,

$$b) \quad z^{(N)}(\eta, x) = \begin{cases} 1 & ; \eta = +\infty \\ 0 & ; \eta = \eta_{II} \end{cases}$$

(B. 29)

The hot boundary in the case of the mixing region is  $\eta_{II} = -\infty$  ; in the case of the boundary layer, the hot boundary is given by  $\eta_{II} = 0$  .

Now temporarily treat  $x$  as a constant, reducing equation B. 29 to a total differential equation as was done in equation B. 9, and define  $\epsilon = dz^{(N)}/d\eta$  . The following differential equation is then obtained.

$$\frac{d\epsilon}{d\eta} + Pr f(\eta) \epsilon = \Sigma(x) Q^{(N-1)}(\eta, x) [f''(\eta)]^{Pr}$$

(B. 30)

Equation B. 30 is a first-order, nonhomogeneous, linear differential equation which has the same integrating factor as equation B. 19; thus from equation B. 23,

$$Q(\eta) = [f''(\eta)]^{-Pr}$$

(B. 31)

is the integrating factor of equation B. 30. Then, using the above expression for the integrating factor, equation B. 30 may be expressed as follows.

$$\frac{d}{d\eta} \left[ \epsilon \{ f''(\eta) \}^{-Pr} \right] = \Sigma(x) Q^{(N-1)}(\eta, x)$$

The above equation is now integrated at constant  $x$  from  $0$  to  $\eta$  and  $\epsilon$  is then replaced by its equivalent,  $d_z^{(N)}/d\eta$ ; thus

$$\left. \begin{aligned} \frac{d_z^{(N)}}{d\eta} &= [f''(\eta)]^{Pr} \left\{ [f''(0)]^{-Pr} \frac{d_z^{(N)}}{d\eta} \Big|_{\eta=0} \right. \\ &\quad \left. + \Sigma(x) \int_0^\eta Q^{(N-1)}(\alpha, x) d\alpha \right\} \end{aligned} \right] \quad (B.32)$$

Equation B.32 is now integrated at constant  $x$  from  $\eta_{II}$  to  $\eta$  and the second boundary condition of equation B.29b is applied. The following result is obtained.

$$\left. \begin{aligned} z^{(N)}(\eta, x) &= \frac{d_z^{(N)}}{d\eta} \Big|_{\eta=0} [f''(0)]^{-Pr} \int_{\eta_{II}}^\eta [f''(\alpha)]^{Pr} d\alpha \\ &\quad + \Sigma(x) \int_{\eta_{II}}^\eta \left\{ [f''(\beta)]^{Pr} \int_0^\beta Q^{(N-1)}(\alpha, x) d\alpha \right\} d\beta \end{aligned} \right] \quad (B.33)$$

Now define,

$$\left. \begin{aligned} \text{a) } R^{(N-1)}(\eta, x) &= \int_{\eta_{II}}^\eta \left\{ [f''(\beta)]^{Pr} \mathcal{L}^{(N-1)}(\beta, x) \right\} d\beta \\ \text{b) } \mathcal{L}^{(N-1)}(\beta, x) &= \int_0^\beta Q^{(N-1)}(\alpha, x) d\alpha \end{aligned} \right] \quad (B.34)$$

Equation B. 33 is now evaluated at  $\eta = +\infty$ , the first boundary condition of equation B. 29b is applied, equation B. 34 is utilized, and the constant of integration in equation B. 33 is determined.

$$\left. \frac{dz^{(N)}}{d\eta} \Big|_{\eta=0} [f''(0)]^{-Pr} = \frac{1 - \Sigma(x) R^{(N-1)}(\infty, x)}{\int_{\eta_{II}}^{\infty} [f''(\alpha)]^{Pr} d\alpha} \right] \quad (B. 35)$$

Equation B. 35 is now substituted into equation B. 33 and equations B. 25, B. 26, and B. 34 are utilized. The following solution to equation B. 29 is then obtained.

$$a) \quad z^{(N)}(\eta, x) = F(\eta) - \Sigma(x) Z^{(N-1)}(\eta, x)$$

where,

$$b) \quad Z^{(N-1)}(\eta, x) = \left[ F(\eta) R^{(N-1)}(\infty, x) - R^{(N-1)}(\eta, x) \right]$$

(B. 36)

An expression for the first derivative with respect to  $\eta$  of  $z^{(N)}(\eta, x)$  is also required in the main body of the text. From equations B. 32, B. 34b, and B. 35 it follows that,

$$\left. \frac{\partial z^{(N)}}{\partial \eta} = [f''(\eta)]^{Pr} \left\{ \frac{1 - \Sigma(x) R^{(N-1)}(\infty, x)}{\int_{\eta_{II}}^{\infty} [f''(\alpha)]^{Pr} d\alpha} + \Sigma(x) Z^{(N-1)}(\eta, x) \right\} \right] \quad (B. 37)$$

The following expressions are now summarized for particular cases.

Note that  $\eta_{II} = -\infty$  and 0 in the mixing region and boundary layer

cases respectively.

Mixing region,  $Pr = Sc \neq 1$ : (Using equations B. 27a, B. 34, and B. 37)

$$\begin{aligned}
 \text{a)} \quad F(\eta) &= \frac{\int_{-\infty}^{\eta} [f''(\alpha)]^{Pr} d\alpha}{\int_{-\infty}^{\infty} [f''(\alpha)]^{Pr} d\alpha} \\
 \text{b)} \quad R^{(N-1)}(\eta, x) &= \int_{-\infty}^{\eta} \left\{ [f''(\alpha)]^{Pr} \mathcal{L}^{(N-1)}(\alpha, x) \right\} d\alpha \\
 \text{c)} \quad \mathcal{L}^{(N-1)}(\eta, x) &= \int_0^{\eta} Q^{(N-1)}(\alpha, x) d\alpha \\
 \text{d)} \quad \frac{\partial z^{(N)}}{\partial \eta} &= [f''(\eta)]^{Pr} \left\{ \frac{1 - \Sigma(x) R^{(N-1)}(\infty, x)}{\int_{-\infty}^{\infty} [f''(\alpha)]^{Pr} d\alpha} + \Sigma(x) \mathcal{L}^{(N-1)}(\eta, x) \right\}
 \end{aligned} \tag{B. 38}$$

Mixing region,  $Pr = Sc = 1$ : (Using equations 72, 83f, 84, B. 34, and B. 37).

$$\begin{aligned}
 \text{a)} \quad F(\eta) = U(\eta) &= \frac{1}{2} f'(\eta) - \frac{\Lambda}{1-\Lambda} \\
 \text{b)} \quad R^{(N-1)}(\eta, x) &= \int_{-\infty}^{\eta} \left\{ f''(\alpha) \mathcal{L}^{(N-1)}(\alpha, x) \right\} d\alpha \\
 \text{c)} \quad \mathcal{L}^{(N-1)}(\eta, x) &= \int_0^{\eta} Q^{(N-1)}(\alpha, x) d\alpha \\
 \text{d)} \quad \frac{\partial z^{(N)}}{\partial \eta} &= \frac{f''(\eta)}{2} \left\{ 1 - \Sigma(x) \left[ R^{(N-1)}(\infty, x) - 2 \mathcal{L}^{(N-1)}(\eta, x) \right] \right\}
 \end{aligned} \tag{B. 39}$$

Boundary layer,  $Pr = Sc \neq 1$ : (Using equations B. 27b, B. 34, and B. 37).

$$\begin{aligned}
 \text{a)} \quad & F(\eta) = \mathcal{D}(Pr) \int_0^\eta [f''(\alpha)]^{Pr} d\alpha \\
 \text{b)} \quad & R^{(N-1)}(\eta, x) = \int_0^\eta \left\{ [f''(\alpha)]^{Pr} \mathcal{L}^{(N-1)}(\alpha, x) \right\} d\alpha \\
 \text{c)} \quad & \mathcal{L}^{(N-1)}(\eta, x) = \int_0^\delta Q^{(N-1)}(\alpha, x) d\alpha \\
 \text{d)} \quad & \frac{\partial \mathcal{L}^{(N)}}{\partial \eta} = [f''(\eta)]^{Pr} \left\{ \mathcal{D}(Pr) - \mathcal{X}(x) \left[ \mathcal{D}(Pr) R^{(N-1)}(\infty, x) - \mathcal{L}^{(N-1)}(\eta, x) \right] \right\} \\
 \text{e)} \quad & \mathcal{D}(Pr) \equiv \left[ \int_0^\infty [f''(\alpha)]^{Pr} d\alpha \right]^{-1} \doteq \left\{ \frac{0.664 Pr^{1/3}}{(1.328)^{Pr}} \right\}
 \end{aligned} \tag{B. 40}$$

where

Boundary layer,  $Pr = Sc = 1$ : (Using equations 72, 83f, 84, B. 34, and B. 37).

$$\begin{aligned}
 \text{a)} \quad & F(\eta) = U(\eta) = \frac{1}{2} f'(\eta) \\
 \text{b)} \quad & R^{(N-1)}(\eta, x) = \int_0^\eta [f''(\alpha) \mathcal{L}^{(N-1)}(\alpha, x)] d\alpha \\
 \text{c)} \quad & \mathcal{L}^{(N-1)}(\eta, x) = \int_0^\delta Q^{(N-1)}(\alpha, x) d\alpha \\
 \text{d)} \quad & \frac{\partial \mathcal{L}^{(N)}}{\partial \eta} = \frac{f''(\eta)}{2} \left\{ 1 - \mathcal{X}(x) \left[ R^{(N-1)}(\infty, x) - 2 \mathcal{L}^{(N-1)}(\eta, x) \right] \right\}
 \end{aligned} \tag{B. 41}$$



APPENDIX C

EVALUATION OF A SUM OF INTEGRALS

From equation 193 of the text:

$$\mathcal{Q}_{l,k}(x) = \sum_{n=l}^k \left\{ d_n \int_{\beta_1}^{\beta_2(x)} \frac{e^{-x}}{x^n} dx \right. \quad (C.1)$$

Denote the integral by,

$$\mathcal{Q}_n(x) = \int_{\beta_1}^{\beta_2(x)} \frac{e^{-x}}{x^n} dx \quad (C.2)$$

then from equations C.1 and C.2 it follows that:

$$\mathcal{Q}_{l,k}(x) = \sum_{n=l}^k d_n \mathcal{Q}_n(x) \quad (C.3)$$

The indefinite integral corresponding to equation C.2 is given as follows in reference 74:

$$\int \frac{e^{-\lambda x}}{x^n} dx = -e^{-\lambda x} \sum_{v=1}^{n-1} \left[ \frac{\lambda^{v-1}}{(n-1; -1; v)} \frac{1}{x^{n-v}} \right] + \frac{\lambda^{n-1}}{(n-1)!} \text{Ei}(\lambda x) + C ; n > 1 \quad (C.4)$$

where Ei(y), the "exponential integral", is a tabulated function<sup>(75)</sup> defined as follows.

$$E_i(y) = \int_{-\infty}^y \frac{e^t}{t} dt \quad \left. \vphantom{\int_{-\infty}^y} \right\} \text{(C.5)}$$

The following relation is given in reference 76:

$$(n-1; -1; v) = (1)^v \binom{n-1}{1} (-1; v) = \frac{(1)^v \Gamma(\binom{n-1}{1} + 1)}{\Gamma(\binom{n-1}{1} - v + 1)}$$

or, more simply, as

$$(n-1; -1; v) = \frac{\Gamma(n)}{\Gamma(n-v)} = \frac{(n-1)!}{(n-1-v)!} \quad \left. \vphantom{\frac{\Gamma(n)}{\Gamma(n-v)}} \right\} \text{(C.6)}$$

The following two definitions are now introduced:

$$G_n(x) \equiv e^{-x} \sum_{v=1}^{n-1} \left[ \frac{(-1)^v (n-1-v)!}{(n-1)! x^{n-v}} \right] + \frac{(-1)^{n-1}}{(n-1)!} E_i(-x) \quad \left. \vphantom{\sum_{v=1}^{n-1}} \right\} \text{(C.7)}$$

and

$$g_{l,k}(x) = \sum_{n=l}^k d_n G_n(x) \quad \left. \vphantom{\sum_{n=l}^k} \right\} \text{(C.8)}$$

Then from equations C.2, C.4, C.6, and C.7:

$$Q_n(x) = G_n[\beta_2(x)] - G_n(\beta_1) \quad \left. \vphantom{G_n[\beta_2(x)]} \right\} \text{(C.9)}$$

Similarly, from equations C.3, C.8, and C.9:

$$\mathcal{G}_{\lambda, k}(\delta) = \mathcal{G}_{\lambda, k}[\beta_2(\delta)] - \mathcal{G}_{\lambda, k}(\beta_1) \quad (\text{C.10})$$

For values of the appropriate parameters (cf. equations 59 and 142b) of practical interest,  $\beta_1$  and  $\beta_2(\delta)$  are both large (i. e.  $\gg 15$ ). The asymptotic expansion for  $\text{Ei}(-\delta)$  may thus be employed. From reference 77:

$$\text{Ei}(-\delta) = -e^{-\delta} \left[ \frac{1}{\delta} - \frac{1}{\delta^2} + \frac{2!}{\delta^3} - \frac{3!}{\delta^4} + \frac{4!}{\delta^5} - \dots \right]$$

or,

$$\text{Ei}(-\delta) = -e^{-\delta} \sum_{N=0}^{|\delta|} \left[ \frac{(-1)^N N!}{\delta^{N+1}} \right] \quad (\text{C.11})$$

where  $|\delta|$  is the first integer smaller than  $\delta$ . The semiconvergent series is terminated at  $|\delta|$  because the terms increase in magnitude with increasing  $N$  when  $N \geq |\delta|$ . Using equation C.11, equation C.7 can be written as follows for large  $\delta$ :

$$G_n(\delta) = \frac{e^{-\delta}}{(n-1)!} \left\{ (-1)^n \sum_{N=0}^{|\delta|} \left[ \frac{(-1)^N N!}{\delta^{N+1}} \right] + \sum_{\nu=1}^{n-1} \left[ \frac{(-1)^\nu (n-\nu-1)!}{\delta^{n-\nu}} \right] \right\}$$

Setting  $N + 1 = n - \nu$  in the first series and simplifying, the following expression can be obtained:

$$G_n(\delta) = \left[ \frac{(-1)^n e^{-\delta}}{(n-1)!} \right] \sum_{N=n}^{|\delta|} \left[ \frac{(-1)^{N-1} (N-1)!}{\delta^N} \right] \quad (\text{C.12})$$

Substituting equation C. 12 into equation C. 8,

$$g_{\lambda, k}(x) = e^{-x} \sum_{n=\lambda}^k \left\{ \frac{(-1)^n d_n}{(n-1)!} \sum_{N=n}^{l+|M|} \left[ \frac{(-1)^{N-1} (N-1)!}{x^N} \right] \right\} \quad (C. 13)$$

Equation C. 13 may be rewritten as follows:

$$g_{\lambda, k}(x) = e^{-x} \sum_{n=\lambda}^k \left\{ \frac{(-1)^n d_n}{(n-1)!} \sum_{N=n}^k \frac{(-1)^{N-1} (N-1)!}{x^N} \right\} + e^{-x} \left\{ \sum_{n=\lambda}^k \frac{(-1)^n d_n}{(n-1)!} \right\} \left\{ \sum_{N=k+1}^{l+|M|} \left[ \frac{(-1)^{N-1} (N-1)!}{x^N} \right] \right\} \quad (C. 14)$$

The second pair of series are now uncoupled and may be taken as the product of two terms. In the first pair of series  $n \leq N \leq k$  ; thus for a given value of N, n can take on the values  $n = \lambda, \lambda + 1, \dots, N$ .

Equation C. 14 may thus be written as follows:

$$g_{\lambda, k}(x) = e^{-x} \left\{ \sum_{n=\lambda}^k \left[ \frac{(-1)^{N-1} (N-1)!}{x^N} q_{\lambda, N} \right] \right\} + q_{\lambda, k} \sum_{N=k+1}^{l+|M|} \left[ \frac{(-1)^{N-1} (N-1)!}{x^N} \right] \quad (C. 15)$$

where,

$$q_{\lambda, M} = \sum_{n=\lambda}^M \left[ \frac{(-1)^n d_n}{(n-1)!} \right] \quad (C. 16)$$

Now define:

$$\beta_N = \begin{cases} (-1)^{N-1} (N-1)! \beta_{2,N} & ; N < k \\ (-1)^{N-1} (N-1)! \beta_{2,k} & ; N \geq k \end{cases} \quad (C.17)$$

then, from equation C.15 - C.17,

$$\mathcal{Q}_{2,k}(s) = e^{-s} \sum_{N=k}^{1+\infty} \left( \beta_N / s^N \right) \quad (C.18)$$

An expression for the desired integral sum is obtained upon substituting equation C.18 into equation C.10:

$$\begin{aligned} \mathcal{Q}_{2,k}(s) &= e^{-\beta_2(s)} \sum_{N=k}^{1+\infty} \frac{\beta_N}{[\beta_2(s)]^N} \\ &\quad - e^{-A} \sum_{N=k}^{1+\infty} \left( \beta_N / \beta_1^N \right) \end{aligned} \quad (C.19)$$

APPENDIX D

DISCUSSION OF COMPUTATIONS

1. Shear-Free Mixing Region: First-Order Kinetics

From equations 112 and 114 of the text,

$$\left. \begin{aligned}
 \text{a) } \quad \bar{\mathcal{L}}(\delta) &= 2 \int_0^{\delta\sqrt{Pr}} \left\{ (1 + \operatorname{erf} \alpha) \exp \left[ \alpha^2 - \frac{\beta_1}{1 - c_2(1 + \operatorname{erf} \alpha)} \right] \right\} d\alpha \\
 \text{b) } \quad \bar{R}(\eta) &= \int_{-\infty}^{\eta\sqrt{Pr}} \left[ e^{-\delta^2} \bar{\mathcal{L}}(\delta) \right] d\delta
 \end{aligned} \right\} \quad (\text{D.1})$$

The integrand of equation D.1a was calculated, using the tabulated error function<sup>(71)</sup>, at increments of  $\Delta\alpha = 0.10$  over the range  $-3 \leq \alpha \leq 3$ . Using Simpson's rule for numerical integration,  $\bar{\mathcal{L}}(\delta)$  was then obtained at increments of  $\Delta(\delta\sqrt{Pr}) = 0.20$  over the range  $-3 \leq \delta\sqrt{Pr} \leq 3$ . Using the calculated values of  $\bar{\mathcal{L}}(\delta)$ , the integrand of equation D.1b was then calculated at intervals of the variable of integration of 0.20. The lower limit of the integral for  $\bar{R}(\eta)$  was approximated by -3.0; this approximation is acceptable because of the influence of the exponential term in the integrand. Simpson's rule was again applied and  $\bar{R}(\eta)$  was obtained at intervals of 0.40 over the range  $-3 \leq \eta \leq 3$ . The quantity  $\bar{R}(\infty)$  is closely approximated by the value  $\bar{R} (+ 3.0)$  by virtue of the rapid decay of  $\bar{\mathcal{L}}(\delta)$  for positive values of the argument and the accentuating decay due to the exponential factor in the integrand. The temperature and concentration profiles and the characteristic stay time are then easily calculated by direct

substitution into equations 114a, 115, and 116. The results of these numerical calculations are presented in figures 4 through 8.

## 2. Shear-Free Mixing Region: Second-Order Kinetics

From equations 119b and 120 of the text:

$$\left. \begin{aligned} \text{a) } \quad \bar{L}(\delta) &= \int_0^{\delta\sqrt{Pr}} \left\{ \frac{(1+\text{erf}\alpha)^2}{1-C_2(1+\text{erf}\alpha)} \right\} \exp\left[\eta^2 - \frac{\beta_1}{1-C_2(1+\text{erf}\alpha)}\right] d\alpha \\ \text{b) } \quad \bar{R}(\eta) &= \int_{-\infty}^{\eta\sqrt{Pr}} \left[ e^{-\delta^2} \bar{L}(\delta) \right] d\delta \end{aligned} \right\} \quad (\text{D. 2})$$

The integrals were numerically evaluated using Simpson's rule; the increments and ranges of integration were the same as for the case of first-order kinetics which was previously discussed. The temperature and concentration profiles and the characteristic stay time were then readily calculated by direct substitution into equations 121 and 122. The variation of the characteristic stay time with static pressure, extent of vitiation, and equivalence ratio were calculated using equations 123, 125, 126, 128, and 132. The results of these numerical calculations are presented in figures 9 through 13.

## 3. Shear-Flow Mixing Region

The dimensionless velocity in the shear-flow mixing region was calculated from equation 145 of the text,

$$\left. \quad U(\eta) = \left( \frac{u - u_{II}}{u_I - u_{II}} \right) = \frac{1}{2} \left[ 1 + \text{erf} \left( \eta \sqrt{\frac{1+\Lambda}{2(1-\Lambda)}} \right) \right] \quad ; \quad \Lambda \neq 1 \right\} \quad (\text{D. 3})$$

for  $-4 \leq \eta \leq 4$  and  $\Lambda$ , the velocity ratio, equal to 0, 0.2, 0.4, 0.6, and 0.8. The results of this calculation are presented in figure 14. The integrals  $\bar{L}(\alpha)$  and  $\bar{R}(\eta)$  were calculated by Simpson's rule as for the previous cases considered; equation D.2 can be simply modified for the shear-flow case by replacing  $\frac{1}{2}(1 + \operatorname{erf} \eta)$  by  $U(\eta)$ , equation D.3 (cf. equations 147, 149, 158). The variation of the characteristic stay time with velocity ratio was obtained by calculating values of the stay time for various velocity ratios, equation 156, and dividing these values by the characteristic stay time for a velocity ratio of unity, equation 109. The results of these calculations are presented in figure 15. The variation of the characteristic stay time with equivalence ratio was readily obtained from equation 159 and is presented in figure 16.

#### 4. Boundary Layer: First-Order Kinetics

From equations 214b, 215a, and 215b of the text:

$$\begin{aligned}
 \text{a)} \quad H(\beta_1) &= 3 \sum_{N=0}^{12} J_N(\beta_1) \\
 \text{b)} \quad L_1(\beta_1) &= - \sum_{N=0}^{12} [N J_N(\beta_1)]
 \end{aligned}
 \tag{D.4}$$

where,

$$\text{c)} \quad J_N(\beta_1) = \left\{ \frac{(-1)^N (N+1)(N+2)!}{6 \beta_1^N} \right\}$$



Evaluating the coefficients,

$$\begin{aligned}
 \text{a) } H(\beta_1) &= 1.00000 - 0.60000 \beta_1^{-1} + 0.36000 \beta_1^{-2} \\
 &\quad - 0.24000 \beta_1^{-3} + 0.18000 \beta_1^{-4} - 0.15120 \beta_1^{-5} \\
 &\quad + 0.14112 \beta_1^{-6} - 0.14515 \beta_1^{-7} + 0.16330 \beta_1^{-8} \\
 &\quad - 0.19958 \beta_1^{-9} + 0.26345 \beta_1^{-10} - 0.37362 \beta_1^{-11} \\
 &\quad + 0.56656 \beta_1^{-12} \\
 \\
 \text{b) } L_1(\beta_1) &= 0.20000 \beta_1^{-1} - 0.24000 \beta_1^{-2} + 0.24000 \beta_1^{-3} \\
 &\quad - 0.24000 \beta_1^{-4} + 0.25200 \beta_1^{-5} - 0.28224 \beta_1^{-6} \\
 &\quad + 0.33869 \beta_1^{-7} - 0.43546 \beta_1^{-8} + 0.59875 \beta_1^{-9} \\
 &\quad - 0.87817 \beta_1^{-10} + 1.36994 \beta_1^{-11} - 2.26664 \beta_1^{-12}
 \end{aligned}
 \tag{D.5}$$

The functions  $H(\beta_1)$  and  $L_1(\beta_1)$  were calculated over the range  $15 \leq \beta_1 \leq 50$  at intervals of  $\Delta \beta_1 = 2.50$ ; the results are presented in figures 23 and 24.

The function  $\bar{R}(\eta)$ , as given by equation 216 of the text, was calculated for values of the parameters corresponding to the decomposition of azomethane; (i. e.,  $T_f = 1650^\circ\text{K}$ ,  $b = 10^{14} \text{ sec}^{-1}$ ,  $E = 50 \text{ Kcal/g-mole}$ ) and with  $T_I = 300^\circ\text{K}$  and  $T_{II} = 1200^\circ\text{K}$ . The interval of the argument  $\eta$  was  $\Delta \eta = 0.10$  and calculations were made over the range  $0 \leq \eta \leq 3$ . The results of the calculations are

presented in figure 27. The characteristic stay time and the temperature and concentration profiles were then calculated from equations 186 and 187 of the text using the previously determined values of the functions  $H(\beta_1)$ ,  $L_1(\beta_1)$ , and  $\bar{R}(\eta)$ . The results of these calculations are presented in figures 26, 28, and 29.

##### 5. Boundary Layer: Second-Order Kinetics

The integrals of equations 223b and 223c were numerically evaluated for  $\phi_0 = 0.2, 0.4, 0.6, \text{ and } 0.8$  using Simpson's rule. An interval of 0.1 was used in evaluating equation 223b and an interval of 0.20 was used in evaluating equation 223c; the range of integration was zero to three. The Blasius derivatives were obtained from Table I. The specie weight fractions in equation 223a were given by equation 221. The functional relation of equation 223 was calculated for the given values of  $\phi_0$ ; the assumption  $\bar{R}(\infty) \doteq \bar{R}(3.0)$ , which is in excellent agreement with calculations, was utilized. The results of these calculations are presented in figure 31. Figure 30 was directly obtained from equation 226.

APPENDIX E

SIMILARITY SOLUTIONS FOR THE SPECIE CONCENTRATIONS  
IN ONE-DIMENSIONAL FLOW SYSTEMS WITH  
CHEMICAL REACTION

The governing relations in the physical plane for one-dimensional flow systems with chemical reaction are compiled in equation 47 of the text; for convenience, these relations are rewritten in equation E. 1 below:

$$a) \quad \frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_0)}{\partial x_0} = 0$$

$$b) \quad \frac{\partial T}{\partial t} + u_0 \frac{\partial T}{\partial x_0} = \frac{1}{Pr} \frac{1}{\rho} \frac{\partial}{\partial x_0} \left( \mu \frac{\partial T}{\partial x_0} \right) + m^* w_{\tilde{n}} (T_f - T_I)$$

$$c) \quad \frac{\partial K_i}{\partial t} + u_0 \frac{\partial K_i}{\partial x_0} = \frac{1}{Sc} \frac{1}{\rho} \frac{\partial}{\partial x_0} \left( \mu \frac{\partial K_i}{\partial x_0} \right) - w_{\tilde{n}} \quad ; \quad i \neq p$$

where: 
$$w_{\tilde{n}} = \begin{cases} w_{\tilde{n}} & i \leq m^* \\ 0 & i = d \end{cases}$$

$$d) \quad K_p = 1 - K_d - \sum_{j=1}^{m^*} K_j$$

$$e) \quad w_{\tilde{n}} = b \left( \frac{p}{RT} \right)^{m^*-1} \exp(-E/RT) \prod_{j=1}^{m^*} K_j$$

(E. 1)

The notation used in the above relations is the same as that employed in the text.

Now introduce the dimensionless temperature  $\bar{y} \equiv T/T_I$  where  $T_I$  is a constant reference temperature. Equation E.1b may then be written as follows:

$$a) \quad \frac{\partial \bar{y}}{\partial t} + u_0 \frac{\partial \bar{y}}{\partial x_0} = \frac{1}{Pr} \frac{1}{\rho} \frac{\partial}{\partial x_0} \left( \mu \frac{\partial \bar{y}}{\partial x_0} \right) + \bar{c}_i w_{\bar{z}}$$

where,

$$b) \quad \bar{c}_i = m^* \left( \frac{T_f - T_I}{T_I} \right)$$

(E.2)

For the case where  $Pr = Sc$ , the following dimensionless variable is introduced:

$$\bar{F}_i(x_0, t) \equiv \begin{cases} \bar{y} + \bar{c}_i K_i & ; \quad i \leq m^* \\ K_i & ; \quad i = d \end{cases}$$

(E.3)

If equations E.1b and E.1c are now added and the above dimensionless variable is introduced, then the N specie concentration continuity relations may be expressed as follows:

$$a) \quad \frac{\partial \bar{F}_i}{\partial t} + u_0 \frac{\partial \bar{F}_i}{\partial x_0} = \frac{1}{Pr} \frac{1}{\rho} \frac{\partial}{\partial x_0} \left( \mu \frac{\partial \bar{F}_i}{\partial x_0} \right) \quad ; \quad i \neq p$$

$$b) \quad K_i = \frac{1}{\bar{c}_i} (\bar{F}_i - \bar{y}) \quad ; \quad i \leq m^*$$

$$c) \quad K_d = \bar{F}_d$$

$$d) \quad K_p = 1 - K_d - \sum_{j=1}^{m^*} K_j$$

(E.4)

The boundary condition and the initial condition appropriate to the variable  $\bar{F}_i$  are readily obtained from the known conditions upon the variables  $\bar{z}$  and  $K_i$  and equation E. 3. The introduction of the variable  $\bar{F}_i$  has not reduced the number of equations to be solved, but has materially reduced the complexity of the specie continuity relation due to the elimination of the reaction term. For a given problem, the definition in equation E. 3 could be modified so that the boundary and initial conditions were independent of the subscript  $i$ ; the  $N-1$  partial differential relations in equation E. 4a would then reduce to a single equation. This is precisely what was accomplished in the text by the introduction of the function defined in equation 67a. Unfortunately, however, this technique cannot be carried out in general but must be individually applied for each mathematical model corresponding to a given class of physical problems; proper account of the appropriate initial and boundary conditions must, of course, be taken.

APPENDIX F

COMBUSTION IN THE LAMINAR BOUNDARY LAYER  
WITH ARBITRARY WALL TEMPERATURE DISTRIBUTION  
AND WITH  $Pr = Sc$

The extension of the Chapman and Rubesin analysis<sup>(78)</sup> for the temperature and velocity profiles in the laminar boundary layer with arbitrary distribution of surface temperature to the case in which an exothermic chemical reaction occurs in the boundary layer is briefly considered in the present Appendix. As in the text, the viscous dissipation function will be deleted as being negligible relative to the heat release due to chemical reaction. The Howarth transformation utilized in the text will be employed rather than the von Mises transformation utilized by Chapman and Rubesin; the end results are equivalent in the present application. In order that the similarity technique of Paragraph III G. 1 may be employed, only the case where  $Pr = Sc$  will be considered.

The governing relations for the laminar boundary layer, expressed in the Howarth plane, are compiled in equation 57 of the text. The following notation is now introduced:

$$\left. \begin{aligned}
 \bar{U} &= u/u_s & \bar{\beta}_1 &= E/R T_s \\
 \bar{V} &= v/u_s & \bar{C}_1 &= m^* \left( \frac{T_f - T_s}{T_s} \right) \\
 \bar{z} &= z/T_s & \bar{C}_3 &= \left( \frac{b}{u_s} \right) \left( \frac{P}{R T_s} \right)^{m^* - 1} \\
 \bar{\Theta}_2 &= \bar{z}^{1-m^*} \prod_{j=1}^{m^*} K_j \exp(-\bar{\beta}_1/\bar{z}) ; \sigma & &= u_s/v
 \end{aligned} \right\} \quad (F. 1)$$

All of the above quantities are dimensionless except for  $\bar{C}_3$  and  $\sigma$  which have the dimension  $\text{cm}^{-1}$ . The subscript I refers to free stream conditions.

Using the notation of equation F. 1, equation 57 may be rewritten as follows:

$$\text{a) } \quad \frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} = 0$$

$$\text{b) } \quad U \frac{\partial U}{\partial x} + V \frac{\partial U}{\partial y} = \frac{1}{\sigma} \frac{\partial^2 U}{\partial y^2}$$

$$\text{c) } \quad U \frac{\partial \bar{z}}{\partial x} + V \frac{\partial \bar{z}}{\partial y} = \frac{1}{Pr\sigma} \frac{\partial^2 \bar{z}}{\partial y^2} + \bar{C}_1 \bar{C}_3 \bar{\Theta}_n(x,y)$$

$$\text{d) } \quad U \frac{\partial K_i}{\partial x} + V \frac{\partial K_i}{\partial y} = \frac{1}{Sc\sigma} \frac{\partial^2 K_i}{\partial y^2} - \bar{C}_3 \bar{\Theta}_n(x,y) \quad ; \quad i \neq p$$

$$\text{e) } \quad K_p = 1 - \epsilon - \sum_{j=1}^{m^*} K_j$$

$$\text{f) } \quad \rho = \frac{\rho M}{R T} \quad ; \quad T = T_I \bar{z}$$

(F. 2)

In the above,  $\epsilon$  denotes the weight fraction of inert diluent in the combustible free stream. For the case of present interest,  $Pr = Sc$ , equation F. 2d can be replaced by a much simpler relation. Multiply equation F. 2d through by  $\bar{C}_1$  and add the resulting expression to equation F. 2c; then

$$a) \quad U \frac{\partial \tau_i}{\partial x} + V \frac{\partial \tau_i}{\partial y} = \frac{1}{\sigma Pr} \frac{\partial^2 \tau_i}{\partial y^2} \quad ; \quad i \neq p$$

where:

$$b) \quad \tau_i = \bar{g} + \bar{c}_i K_i$$

(F. 3)

The Blasius transformation is now utilized (cf. Section IIH). Equations F. 2 and F. 3 can then be summarized as follows in the  $\eta$  ,  $x$  plane.

$$a) \quad f'''(\eta) + f(\eta)f''(\eta) = 0$$

$$b) \quad \frac{\partial^2 \bar{g}}{\partial \eta^2} + Pr f(\eta) \frac{\partial \bar{g}}{\partial \eta} = 2 Pr X f'(\eta) \frac{\partial \bar{g}}{\partial x} - 4 Pr X \bar{c}_1 \bar{c}_3 \bar{\theta}_2(\eta, X)$$

$$c) \quad \frac{\partial^2 \tau_i}{\partial \eta^2} + Pr f(\eta) \frac{\partial \tau_i}{\partial \eta} = 2 Pr X f'(\eta) \frac{\partial \tau_i}{\partial x}$$

(F. 4)

$$d) \quad u = u_x U = \frac{1}{2} f'(\eta) u_x$$

$$e) \quad K_i = \frac{1}{\bar{c}_i} (\tau_i - \bar{g}) \quad ; \quad i \neq p$$

$$f) \quad K_p = 1 - \epsilon + \frac{1}{\bar{c}_1} \left[ m^* \bar{g} - \sum_{i=1}^{m^*} \tau_i \right]$$

$$g) \quad S = \frac{PM}{QT}$$



The boundary conditions corresponding to the above equations are as follows:

$$\begin{array}{l}
 \text{a) } f'(\eta) = \begin{cases} 2 & ; \eta = \infty \\ 0 & ; \eta = 0 \end{cases} \\
 \text{b) } \bar{T}_i(\eta, x) = \begin{cases} 1 & ; \eta = \infty \\ \bar{T}_{i_0}(x) & ; \eta = 0 \end{cases} \\
 \text{c) } \tau_{i_0}(\eta, x) = \begin{cases} a_i \equiv 1 + \bar{c}_i K_{i_0} & ; \eta = \infty \\ \tau_{i_0}(x) \equiv \bar{T}_{i_0}(x) + \bar{c}_i K_{i_0}(x) & ; \eta = 0 \end{cases}
 \end{array} \quad (F.5)$$

The symbols  $\bar{T}_{i_0}(x)$  and  $K_{i_0}(x)$  respectively denote the dimensionless temperature and the i'th specie weight fraction along the wall. Note that the latter must be intimately related to the former.

The solution to equation F. 4a with the boundary conditions of F.5a is the classic Blasius solution<sup>(60)</sup>; a more recent solution by Emmons and Leigh<sup>(70)</sup> which was obtained on modern high speed computing equipment is tabulated in Table I.

The solution of equation F. 4c with the boundary conditions of F.5c is obtained, in general form, upon solving the following partial differential equation:

$$a) \quad \frac{\partial^2 F}{\partial \eta^2} + P_r f(\eta) \frac{\partial F}{\partial \eta} - 2 P_r x f'(\eta) \frac{\partial F}{\partial x} = 0$$

with,

$$b) \quad F(\eta, x) = \begin{cases} a & ; \eta = \infty \\ F_0(x) & ; \eta = 0 \end{cases}$$

(F.6)

Equation F.6a is a linear, second-order homogeneous, partial differential equation. The standard mathematical technique of separation of variables is thus applicable. Variables are separated in the form,

$$F_2(\eta, x) = \psi_2(x) \mathcal{J}_2(\eta)$$

(F.7)

Substitution of equation F.7 into equation F.6a followed by the separation of variables yields the following expression:

$$2 P_r x \left[ \frac{\psi_2'(x)}{\psi_2(x)} \right] = [f'(\eta) \mathcal{J}_2(\eta)]^{-1} [\mathcal{J}_2''(\eta) + P_r f(\eta) \mathcal{J}_2'(\eta)]$$

Since the left hand side of the above expression is independent of the right hand side, and vice versa, both sides must be equal to a constant, say  $2 P_r \lambda$  ; thus

$$a) \quad \frac{d\psi_\lambda}{\psi_\lambda} = \lambda \frac{dx}{x} \quad (F.8)$$

$$b) \quad \mathcal{J}_\lambda''(\eta) + P_r f(\eta) \mathcal{J}_\lambda'(\eta) - 2P_r \lambda f'(\eta) \mathcal{J}_\lambda(\eta) = 0$$

The solution to equation F. 8a, neglecting the constant of integration, is,

$$\psi_\lambda(x) = x^\lambda \quad (F.9)$$

The boundary conditions most convenient to impose on equation F. 8b are

$$\mathcal{J}_\lambda(\eta) = \begin{cases} a & ; \eta = \infty \\ 1 & ; \eta = 0 \end{cases} \quad (F.10)$$

The function  $\mathcal{J}_\lambda(\eta)$  which satisfies equations F. 8b and F. 10 can be obtained by straightforward numerical solutions (cf. reference 78).

Then, using the principle of superposition, equations F. 6, F. 7, and F. 9 can be combined to yield the following expression:

$$F(\eta, x) = \sum_{\lambda=0}^{\infty} A_\lambda x^\lambda \mathcal{J}_\lambda(\eta) \quad (F.11)$$

where the coefficients  $A_\lambda$  are given by,

$$\sum_{\lambda=0}^{\infty} A_\lambda x^\lambda = F_0(x) \quad (F.12)$$

Note that the coefficients  $A_\lambda$  are simply the coefficients for the Taylor series expansion of the known distribution along the wall.

Comparing equations F.4c, F.5c, and F.6 and using the above two equations it follows that,

$$a) \quad \tau_{\lambda_0}(\eta, x) = \sum_{\lambda=0}^{\infty} A_\lambda x^\lambda \bar{\theta}_\lambda(\eta)$$

where,

$$b) \quad \sum_{\lambda=0}^{\infty} A_\lambda x^\lambda = \tau_{\lambda_0}(x) \equiv \bar{\theta}_0(x) + \bar{C}_1 K_{\lambda_0}(x) \tag{F.13}$$

and  $\bar{\theta}_\lambda(\eta)$  is given by,

$$c) \quad \begin{aligned} \bar{\theta}_\lambda''(\eta) + Pr f'(\eta) \bar{\theta}_\lambda'(\eta) - 2Pr \lambda f'(\eta) \bar{\theta}_\lambda(\eta) &= 0 \\ \bar{\theta}_\lambda(\eta) &= \begin{cases} 1 + \bar{C}_1 K_{\lambda_0} & ; \eta = \infty \\ 1 & ; \eta = 0 \end{cases} \end{aligned}$$

The energy equation, equation F.4b, is the only equation which remains to be solved. The iteration procedure employed in previous considerations of combustion in the laminar boundary layer (cf. Part V) will be utilized. Define  $\bar{\theta}_\lambda^{(0)}(\eta, x)$  as the dimensionless temperature profile in the absence of chemical reaction but with the wall temperature distribution of interest. Setting the reaction term, the last term, in equation F.4b equal to zero and using equation F.5b, it follows that,

$$a) \quad \frac{\partial^2 \bar{z}^{(0)}}{\partial \eta^2} + Pr f(\eta) \frac{\partial \bar{z}^{(0)}}{\partial \eta} = 2 Pr x f'(\eta) \frac{\partial \bar{z}^{(0)}}{\partial x}$$

with:

$$b) \quad \bar{z}^{(0)}(\eta, x) = \begin{cases} 1 & ; \eta = \infty \\ \bar{z}_0(x) & ; \eta = 0 \end{cases}$$

(F. 14)

The above equation is a special case of equation F. 6 and the solution is given in equations F. 11 and F. 12; thus,

$$a) \quad \bar{z}^{(0)}(\eta, x) = \sum_{\lambda=0}^{\infty} A_{\lambda} x^{\lambda} \bar{z}_{\lambda}(\eta)$$

where,

$$b) \quad \sum_{\lambda=0}^{\infty} A_{\lambda} x^{\lambda} = \bar{z}_0(x)$$

(F. 15)

and  $\bar{z}_{\lambda}(\eta)$  is given by,

$$c) \quad \bar{z}_{\lambda}''(\eta) + Pr f(\eta) \bar{z}_{\lambda}'(\eta) - 2 Pr \lambda f'(\eta) \bar{z}_{\lambda}(\eta) = 0$$

$$\bar{z}_{\lambda}(\eta) = \begin{cases} 1 & ; \eta = \infty \\ 1 & ; \eta = 0 \end{cases}$$

The N'th approximation to the dimensionless temperature in a boundary layer in which chemical reaction is occurring is then given

by the following partial differential equation (cf. equations F. 1, F. 4b, F. 4e, F. 16 and Part V. of the text):

$$\begin{aligned}
 \text{a) } \quad \frac{\partial^2 \bar{z}^{(N)}}{\partial \eta^2} + P r f(\eta) \frac{\partial \bar{z}^{(N)}}{\partial \eta} - 2 P r X f'(\eta) \frac{\partial \bar{z}^{(N)}}{\partial X} \\
 = -4 P r X \bar{c}_1 \bar{c}_3 \bar{\Theta}_{\sim}^{(N-1)}(\eta, X)
 \end{aligned}$$

where,

$$\begin{aligned}
 \text{b) } \quad \bar{\Theta}_{\sim}^{(N-1)}(\eta, X) = \left[ \bar{z}^{(N-1)}(\eta, X) \right]^{1-m^*} \exp \left[ \frac{-\bar{\beta}_1}{\bar{z}^{(N-1)}(\eta, X)} \right] \cdot \\
 \bar{c}_1^{-m^*} \prod_{j=1}^{m^*} [\tau_j - \bar{z}^{(N-1)}]
 \end{aligned} \tag{F. 16}$$

and,

$$\text{c) } \quad \bar{z}^{(N)}(\eta, X) = \begin{cases} 1 & ; \eta = \infty \\ \bar{z}_0(X) & ; \eta = 0 \end{cases}$$

Equation F. 16a is a linear, second-order, nonhomogeneous partial differential equation. By virtue of its linearity, the solution may be obtained by adding a particular solution of the nonhomogeneous equation to a solution of the homogeneous equation. Thus,

$$\bar{z}^{(N)}(\eta, X) = \bar{z}_p^{(N)}(\eta, X) + \bar{z}_h(\eta, X) \tag{F. 17}$$

Note that the solution to the homogeneous equation is the same for all iterations.

In the above expression,  $z_p^{(N)}(\eta, x)$  and  $z_H(\eta, x)$  denote the particular and the homogeneous solution respectively. The boundary conditions to be assigned to the particular and to the homogeneous solution may be chosen subject only to the conditions that

$$z_p^{(N)}(\eta, x) + z_H(\eta, x) = \begin{cases} 1 & ; \eta = \infty \\ \bar{z}_0(x) & ; \eta = 0 \end{cases}$$

The following boundary conditions will prove to be convenient.

$$\text{a) } z_p^{(N)}(\eta, x) = \begin{cases} 1 & ; \eta = \infty \\ 0 & ; \eta = 0 \end{cases}$$

$$\text{b) } z_H(\eta, x) = \begin{cases} 0 & ; \eta = \infty \\ \bar{z}_0(x) & ; \eta = 0 \end{cases}$$

(F.18)

The homogeneous solution has already been obtained in general form, cf. equations F.6, F.8b, F.10, F.11, and F.12. Thus,

$$a) \quad \mathcal{Z}_H(\eta, x) = \sum_{\lambda=0}^{\infty} A_{\lambda} x^{\lambda} \mathcal{Z}_{\lambda}(\eta)$$

where,

$$b) \quad \sum_{\lambda=0}^{\infty} A_{\lambda} x^{\lambda} = \bar{\mathcal{Z}}_0(x) \quad (F.19)$$

and,

$$c) \quad \mathcal{Z}_{\lambda}''(\eta) + Pr f'(\eta) \mathcal{Z}_{\lambda}'(\eta) - 2Pr \lambda f'(\eta) \mathcal{Z}_{\lambda}(\eta) = 0$$

$$\mathcal{Z}_{\lambda}(\eta) = \begin{cases} 0 & ; \eta = \infty \\ 1 & ; \eta = 0 \end{cases}$$

An exact particular solution cannot be obtained. However, a satisfactory solution can be obtained by simply approximating  $\partial \mathcal{Z}_p^{(N)} / \partial x$  by  $\partial \mathcal{Z}_p^{(N-1)} / \partial x$ . Now introduce the following dimensionless variables,

$$a) \quad Q_p^{(N-1)}(\eta, x) = 2Pr [f''(\eta)]^{-Pr} \left\{ \frac{f'(\eta)}{\bar{c}_1 \bar{c}_3} \frac{\partial \mathcal{Z}_p^{(N-1)}}{\partial x} - 2 \bar{\Theta}_{2p}^{(N-1)}(\eta, x) \right\} \quad (F.20)$$

$$b) \quad \bar{X}(x) = \bar{c}_1 \bar{c}_3 x$$



Using equations F. 16a, F. 17, F. 18a, and F. 20, the following partial differential expression for the particular solution can be obtained.

$$a) \quad \frac{\partial^2 z_p^{(N)}}{\partial \eta^2} + P_r f(\eta) \frac{\partial z_p^{(N)}}{\partial \eta} = \bar{X}(x) [f''(\eta)]^{P_r} Q_p^{(N-1)}(\eta, x) \quad (F. 21)$$

with, 
$$z_p^{(N)}(\eta, x) = \begin{cases} 1 & ; \eta = \infty \\ 0 & ; \eta = 0 \end{cases}$$

Equation F. 21 is in the identical form of the energy equation for combustion in a laminar boundary layer with a constant wall temperature; this equation was discussed in Section V B and the solution is carried out in Appendix B-4. The solution is as follows,

$$z_p^{(N)}(\eta, x) = F(\eta) - \bar{X}(x) z_p^{(N-1)}(\eta, x) \quad (F. 22)$$

where,

$$\begin{aligned}
 \text{a)} \quad Z_p^{(N-1)} &= [F(\eta) R_p^{(N-1)}(\infty, x) - R_p^{(N-1)}(\eta, x)] \\
 \text{b)} \quad F(\eta) &= \mathcal{B}(Pr) \int_0^\eta [f''(\alpha)]^{Pr} d\alpha \\
 \text{c)} \quad \mathcal{B}(Pr) &\equiv \left[ \int_0^\infty [f''(\alpha)]^{Pr} d\alpha \right]^{-1} = \left\{ \frac{0.664 Pr^{1/3}}{(1.328) Pr} \right\} \\
 \text{d)} \quad R_p^{(N-1)}(\eta, x) &= \int_0^\eta \left\{ [f''(\delta)]^{Pr} \mathcal{Z}_p^{(N-1)}(\delta, x) \right\} d\delta \\
 \text{e)} \quad \mathcal{Z}_p^{(N-1)}(\eta, x) &= \int_0^\delta Q_p^{(N-1)}(\alpha, x) d\alpha
 \end{aligned} \tag{F. 23}$$

The N'th approximation to the dimensionless temperature in a laminar boundary layer with exothermic chemical reaction and with an arbitrary surface distribution of temperature may now be written as follows (cf. equations F. 17, F. 19, and F. 22):

$$\bar{z}^{(N)}(\eta, x) = F(\eta) - \bar{\Sigma}(x) Z_p^{(N-1)}(\eta, x) + \sum_{\lambda=0}^{\infty} A_\lambda x^\lambda \mathcal{Z}_\lambda(\eta) \tag{F. 24}$$

The various terms in the above expression are defined in equations F. 19, F. 20, and F. 22. The N'th approximation to the specie concentrations can be obtained by substituting equations F. 13 and F. 24 into equations F. 4e and F. 4f.

## APPENDIX G

### CHEMICAL REACTION IN THE HYPERSONIC BOUNDARY LAYER WITH $Pr = Sc = 1$

By virtue of the similarity solutions for the specie concentration relations, the analysis of the text can readily be extended to the technically important problem of dissociation and recombination in the hypersonic boundary layer\*. In order to employ the similarity solutions, however, the analysis must be restricted to the special case where  $Pr = Sc = 1$ . Needless to say, this assumption will lead to results which are not quantitatively reliable; the qualitative results, however, should be acceptable.

The governing relations in the Howarth (x, y) plane for low speed boundary layer flow with a one-step unopposed chemical reaction are presented in equation 57 of the text. In order to modify these

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\* In almost all practical cases, a body moving at hypersonic speeds will have a detached shock wave due to the bluntness of the nose or of the leading edge; nose bluntness is almost a certainty: as a result of the melting of a sharp nose if not by logical design. Because of the extreme temperature rise through the shock wave, the flow field behind the shock will initially be in an almost completely dissociated state. This is indeed a fortunate occurrence for the endothermic dissociation reaction markedly reduces the thermal energy of the flow field about the body and thus greatly reduces the heat flux to the body. The flow of heat to the relatively cool body, however, results in lower temperatures in the boundary layer and at these lower temperatures the reverse or exothermic recombination reaction can dominate the desirable endothermic dissociation reaction. Thus the "problem of dissociation in the hypersonic boundary layer", often referred to in the literature, is in reality a problem of recombination and of dissociation.

relations for application to the problem of present interest, chemical reaction in the hypersonic boundary layer, two changes must be made: (1) the viscous dissipation term, neglected in the low speed case, must be added to the right hand side of the energy balance relation, equation 57c and (2) the reaction term, equation 57f, must be generalized for application to an opposed reaction.

By virtue of the conventional boundary layer assumptions<sup>(54)</sup>, the viscous dissipation function, given in equation 14, can be approximated as follows in the physical  $(x_o, y_o)$  plane:

$$\bar{\Phi}(x_o, y_o) = \left( \frac{\partial u_o}{\partial y_o} \right)^2 \quad (G. 1)$$

Using equations 50 and 55, the equivalent expression in the Howarth  $(x, y)$  plane is as follows:

$$\bar{\Phi}(x, y) = \left( \frac{\rho}{\rho_I} \right)^2 \left( \frac{\partial u}{\partial y} \right)^2 \quad (G. 2)$$

The viscous dissipation term which is to be added to the right hand side of the low speed form of the energy balance relation, equation 57c, is obtained upon comparing the last expression of page 35 with equation 57c and using equations G. 2 and 35; thus

$$\frac{\mu}{\rho c_p} \bar{\Phi}(x, y) = \left( \frac{\mu \rho}{c_p \rho_I^2} \right) \left( \frac{\partial u}{\partial y} \right)^2 = \frac{\nu}{c_p} \left( \frac{\partial u}{\partial y} \right)^2 \quad (G. 3)$$

The energy balance relation appropriate for high speed flow with

chemical reaction is obtained from equations 34, 57c, and G. 3.

$$u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \frac{v}{Pr} \frac{\partial^2 T}{\partial y^2} + \frac{v}{C_p} \left( \frac{\partial u}{\partial y} \right)^2 + \overline{\Delta H} \overline{w}_r(x,y) \quad (G. 4)$$

The left hand side of the preceding equation relates to the convection of heat; the terms on the right hand side of the equation relate to the conduction of heat, the conversion of kinetic energy to heat by viscous dissipation, and the heat release due to chemical reaction respectively.

The symbol  $\overline{\Delta H}$  is defined in equation 33. The reaction term given in equation 57f for an unopposed reaction of the form of equation 25 can be readily generalized to an opposed reaction as follows (cf. reference 39):

$$\overline{w}_r(x,y) = b \left( \frac{p}{RT} \right)^{m^*-1} \left[ 1 - \left( \frac{K_p}{K_{pe}} \right)^{m^*} \prod_{j=1}^{m^*} \left( \frac{K_{je}}{K_j} \right) \right] \cdot \prod_{j=1}^{m^*} K_j \exp(-E/RT) \quad (G.5)$$

The subscript e refers to the equilibrium value under the local conditions of temperature and pressure.

Using equations 34, G. 4, and G. 5, the low speed relations of equation 57c can be modified to the following form appropriate for high speed flow systems:

$$a) \quad \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

$$b) \quad u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = v \frac{\partial^2 u}{\partial y^2}$$

$$c) \quad u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \frac{v}{Pr} \frac{\partial^2 T}{\partial y^2} + \frac{v}{c_p} \left( \frac{\partial u}{\partial y} \right)^2 + \overline{\Delta H} \overline{w}_r(x,y) \quad (G.6)$$

$$d) \quad u \frac{\partial K_i}{\partial x} + v \frac{\partial K_i}{\partial y} = \frac{v}{Sc} \frac{\partial^2 K_i}{\partial y^2} - \overline{w}_2(x,y) \quad ; \quad i \neq p$$

$$e) \quad K_p = 1 - \epsilon - \sum_{j=1}^{m^*} K_j$$

The symbol  $\epsilon$  denotes the weight fraction of inert gas in the flow system; at very high Mach numbers  $\epsilon$  will be very close to zero since the major constituents of air will be dissociating and recombining.

The following notation is now introduced. The subscripts I and II refer to the conditions just behind the shock and on the surface of the body respectively.

$$\begin{aligned}
 U &= u/u_I & G_i &= \bar{c}_i [K_i - K_{iII}] \\
 V &= v/u_I & \sigma &= u_I/v \\
 \beta &= \left( \frac{T_{II} - T_I}{T_{II} - T_I} \right) & \beta_1 &= (E/R T_{II}) \\
 \bar{c}_1 &= \left( \frac{\Delta H}{T_{II} - T_I} \right) & C_2 &= \left( \frac{T_{II} - T_I}{2 T_{II}} \right) \\
 C_3 &= \left( \frac{b}{u_I} \right) \left( \frac{p}{R T_{II}} \right)^{m^* - 1} & C_4 &= \frac{U u_I}{c_p (T_{II} - T_I)} \\
 \bar{\Theta}_\lambda(x, y) &= [1 - 2C_2 \beta]^{1 - m^*} \exp \left[ \frac{-\beta_1}{1 - 2C_2 \beta} \right] \cdot \\
 &\quad \prod_{j=1}^{m^*} \left\{ K_j \left[ 1 - \left( \frac{K_p}{K_e} \right)^{m^*} \prod_{j=1}^{m^*} (K_{je}/K_j) \right] \right\}
 \end{aligned} \tag{G.7}$$

Using the above notation, the relations of equation G.6 can be expressed as follows:

$$\begin{aligned}
 \text{a)} \quad & \frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} = 0 \\
 \text{b)} \quad & U \frac{\partial U}{\partial x} + V \frac{\partial U}{\partial y} = \frac{1}{\sigma} \frac{\partial^2 U}{\partial y^2} \\
 \text{c)} \quad & U \frac{\partial \beta}{\partial x} + V \frac{\partial \beta}{\partial y} = \frac{1}{\sigma Pr} \frac{\partial^2 \beta}{\partial y^2} - C_4 \left( \frac{\partial U}{\partial y} \right)^2 - \bar{c}_1 C_3 \bar{\Theta}_\lambda(x, y) \\
 \text{d)} \quad & U \frac{\partial G_i}{\partial x} + V \frac{\partial G_i}{\partial y} = \frac{1}{\sigma Sc} \frac{\partial^2 G_i}{\partial y^2} - \bar{c}_1 C_3 \bar{\Theta}_\lambda(x, y) \quad ; i \neq P \\
 \text{e)} \quad & K_p = 1 - \epsilon - \sum_{j=1}^{m^*} K_j \quad ; K_i = K_{iII} + \frac{G_i}{\bar{c}_i} \quad ; i \neq P
 \end{aligned} \tag{G.8}$$

Now introduce the assumption  $Pr = Sc$  and subtract equation G. 8d from equation G. 8c; thus

$$\begin{aligned} U \frac{\partial}{\partial x} (z - G_i) + \nabla \frac{\partial}{\partial y} (z - G_i) &= \frac{1}{\sigma Pr} \frac{\partial^2}{\partial y^2} (z - G_i) \\ &\quad - C_4 \left( \frac{\partial \sigma}{\partial y} \right)^2 ; i \neq P \end{aligned} \quad \left. \vphantom{\frac{\partial}{\partial x}} \right\} \text{(G. 9)}$$

Define:

$$\begin{aligned} \text{a)} \quad F_i(x, y) &\equiv \left( \frac{z - G_i}{z_I - G_{iI}} \right) = \left\{ \frac{z - \bar{c}_i (K_{iI} - K_{iII})}{1 - \bar{c}_i (K_{iI} - K_{iII})} \right\} \\ \text{b)} \quad \alpha_i &= \frac{C_4 \sigma}{1 - \bar{c}_i (K_{iI} - K_{iII})} \end{aligned} \quad \left. \vphantom{\frac{\partial}{\partial x}} \right\} \text{(G. 10)}$$

and then divide equation G. 9 through by  $[1 - \bar{c}_i (K_{iI} - K_{iII})]$  ; then, using the above definitions,

$$\begin{aligned} \text{a)} \quad U \frac{\partial F_i}{\partial x} + \nabla \frac{\partial F_i}{\partial y} &= \frac{1}{\sigma Pr} \frac{\partial^2 F_i}{\partial y^2} - \frac{\alpha_i}{\sigma} \left( \frac{\partial \sigma}{\partial y} \right)^2 ; i \neq P \\ \text{b)} \quad K_i &= K_{iII} + F_i (K_{iI} - K_{iII}) - \frac{1}{\bar{c}_i} (F_i - z) ; i \neq P \end{aligned} \quad \left. \vphantom{\frac{\partial}{\partial x}} \right\} \text{(G. 11)}$$

By virtue of the similarity for  $Pr = Sc$ , equation G. 6d can be replaced by the simpler relations of equation G. 11.



Equation G. 11a can be solved in a manner analogous with that used by Buseman<sup>(79)</sup> in solving for the temperature profile in a compressible boundary layer. Assume that  $F(x, y)$  is dependent only upon  $\bar{U}$  ; thus  $F_{\lambda}(x, y) = F_{\lambda}(\bar{U})$ . Equation G. 11a can then be written as follows:

$$Pr \left[ \bar{U} \frac{\partial \bar{U}}{\partial x} + \bar{V} \frac{\partial \bar{U}}{\partial y} - \frac{1}{\sigma Pr} \frac{\partial^2 \bar{U}}{\partial y^2} \right] \frac{dF_{\lambda}}{d\bar{U}} = \frac{1}{\sigma} \left( \frac{\partial \bar{U}}{\partial y} \right)^2 \left[ \frac{d^2 F_{\lambda}}{d\bar{U}^2} - \alpha_{\lambda} Pr \right]$$

If the Prandtl number is set equal to unity, the left hand side of the preceding relation reduces to zero by virtue of the momentum relation, equation G. 8b; then since  $\left( \frac{\partial \bar{U}}{\partial y} \right) \neq 0$  , it follows that,

$$\frac{d^2 F_{\lambda}}{d\bar{U}^2} = \alpha_{\lambda}$$

and thus,

$$F_{\lambda}(\bar{U}) = \frac{\alpha_{\lambda}}{2} \bar{U}^2 + a\bar{U} + b \tag{G. 12}$$

Since  $F_{\lambda}(\bar{U})$  has the same boundary conditions as  $\bar{U}$  (equal to unity just behind the shock wave and equal to zero along the surface of the body),

$$\left. \begin{aligned} \frac{\alpha_{\lambda}}{2} + a + b &= 1 \\ b &= 0 \end{aligned} \right\}$$

thus,

$$F_{\lambda}(\bar{U}) = \bar{U} \left[ 1 - \frac{\alpha_{\lambda}}{2} (1 - \bar{U}) \right] \tag{G. 13}$$

Note that equation G. 13 reduces to the proper form for the low speed case; when the viscous dissipation function is set equal to zero,  $\alpha_i$  also is equal to zero and  $F_i(\sigma) = \sigma$  as was previously found in the low speed case treated in the text; cf. equation 72.

Using equations G. 8c, G. 11, and G. 12, the specie weight fractions can now be expressed in terms of the dimensionless temperature and the dimensionless streamwise velocity.

$$\left. \begin{aligned} \text{a)} \quad K_i &= K_{i, \text{II}} + F(\sigma) [K_{i, \text{I}} - K_{i, \text{II}}] - \frac{1}{C_1} [F(\sigma) - \beta] \\ &\qquad \qquad \qquad ; i \neq p \\ \text{b)} \quad K_p &= 1 - \epsilon - \sum_{j=1}^{m^*} K_j \\ \text{c)} \quad F_i(\sigma) &= \sigma \left[ 1 - \frac{\alpha_i}{2} (1 - \sigma) \right] \end{aligned} \right\} \quad (\text{G. 14})$$

The relations which remain to be solved, equations G. 8a, b, c, can most conveniently be considered in the Blasius  $(\eta, x)$  plane used in the analysis of the text. These relations can be expressed as follows in the  $\eta, x$  plane; cf. the Blasius transformation of Section II H.

$$\left. \begin{aligned} \text{a)} \quad f'''(\eta) + f(\eta)f''(\eta) &= 0 \\ \text{b)} \quad \frac{\partial^2 \bar{c}_2}{\partial \eta^2} + f(\eta) \frac{\partial \bar{c}_2}{\partial \eta} &= 2xf'(\eta) \frac{\partial \bar{c}_2}{\partial x} + C_4 \sigma \left[ \frac{f''(\eta)}{2} \right]^2 \\ &\quad + 4x\bar{c}_1 C_3 \bar{\Theta}_\infty(\eta, x) \end{aligned} \right\} \quad (\text{G. 15})$$

Negligible error will be made if the conditions just behind the shock are satisfied at  $\eta_I = \infty$ . The solution to equation G. 15a is then the classic Blasius solution which has been previously discussed (cf. Part V) and which is tabulated in Table I. Equation G. 15b will be solved in the same iterative manner as utilized heretofore. Define the following dimensionless quantities:

$$\begin{aligned}
 \text{a)} \quad Q^{(N)}(\eta, x) &= [f''(\eta)]^{-1} \left\{ \frac{2f'(\eta)}{\bar{c}_1 \bar{c}_3} \frac{\partial z^{(N)}}{\partial x} + \frac{\sigma C_a}{4\bar{c}_1 \bar{c}_3 x} \left[ \frac{f''(\eta)}{2} \right]^2 \right. \\
 &\quad \left. + 4\bar{\Theta}_{\sim}^{(N)}(\eta, x) \right\} \\
 \text{b)} \quad \bar{X}(x) &= \bar{c}_1 \bar{c}_3 x
 \end{aligned} \tag{G. 16}$$

Then the N'th approximation to the dimensionless temperature in the hypersonic boundary layer with chemical reaction is given by,

$$\frac{\partial^2 z^{(N)}}{\partial \eta^2} + f(\eta) \frac{\partial z^{(N)}}{\partial \eta} = \bar{X}(x) f''(\eta) Q^{(N-1)}(\eta, x) \tag{G. 17}$$

with,

$$z^{(N)}(\eta, x) = \begin{cases} 1 & ; \eta = \infty \\ 0 & ; \eta = 0 \end{cases}$$

The above equation is equivalent in form to the corresponding energy equation for the low speed flow case, cf. Part V. The solution to this equation, which is carried out in Appendix B-4, is as follows:

$$a) \quad z^{(N)}(\eta, x) = z(\eta) - \bar{X}(x) z^{(N-1)}(\eta, x)$$

where,

$$b) \quad z(\eta) = \frac{1}{2} f'(\eta)$$

$$c) \quad R^{(N-1)}(\eta, x) = \int_0^\eta \left\{ f''(\theta) z^{(N-1)}(\theta, x) \right\} d\theta$$

$$d) \quad z^{(N-1)}(\eta, x) = \int_0^x Q^{(N-1)}(\alpha, x) d\alpha$$

$$e) \quad z^{(N-1)}(\eta, x) = \left[ z(\eta) R^{(N-1)}(\infty, x) - R^{(N-1)}(\eta, x) \right]$$

(G. 18)

As in the text, the basis for the iteration will be the dimensionless temperature profile in the absence of chemical reaction, denoted by  $z^{(0)}(\eta, x)$ . The governing relation for this quantity, expressed in  $\eta, x$  coordinates, is given by equation G. 15a with the reaction term, the last term, set equal to zero. The resulting partial differential equation can be solved by the technique of separating variables in much the same manner as was employed in Appendix F. However, the solution may be carried out in a much simpler manner in the  $x, y$  plane. Thus, setting the reaction term in equation G. 8c equal to zero, the following governing relation for the dimensionless temperature in the absence of chemical reaction is obtained.

$$a) \quad U \frac{\partial z^{(0)}}{\partial x} + V \frac{\partial z^{(0)}}{\partial y} - \frac{1}{\sigma} \frac{\partial^2 z^{(0)}}{\partial y^2} = -C_4 \left( \frac{\partial U}{\partial y} \right)^2$$

with,

$$b) \quad z^{(0)}(x, y) = \begin{cases} 1 & ; \sigma = 1 \\ 0 & ; \sigma = 0 \end{cases}$$

(G. 19)

Now, following Busemann<sup>(79)</sup>, assume  $z^{(0)} = z^{(0)}(\sigma)$  ; equation G. 19a then reduces to the following expression.

$$\left[ U \frac{\partial U}{\partial x} + V \frac{\partial U}{\partial y} - \frac{1}{\sigma} \frac{\partial^2 U}{\partial y^2} \right] \frac{dz^{(0)}}{d\sigma} = \frac{1}{\sigma} \left( \frac{\partial U}{\partial y} \right)^2 \left[ \frac{d^2 z^{(0)}}{d\sigma^2} - C_4 \sigma \right]$$

The left hand side is equal to zero by virtue of the momentum relation, equation G. 8b; thus

$$\frac{d^2 z^{(0)}}{d\sigma^2} = C_4 \sigma$$

or,

$$z^{(0)}(\sigma) = \frac{C_4 \sigma}{2} \sigma^2 + a\sigma + b \tag{G. 20}$$

Application of the boundary conditions of equation G. 19b to equation G. 20 yields the following expression.

Using the appropriate definitions from equation G.7 and noting that  $\bar{T} = \frac{1}{2}f'(\eta)$ , the dimensionless temperature in the absence of chemical reaction can be expressed as follows:

$$z^{(0)}(\bar{T}) = z^{(0)}(\eta) = \frac{f'(\eta)}{2} \left[ 1 - \frac{u_{\infty}^2}{4c_p(\bar{T}_{\infty} - \bar{T}_{\infty})} \{2 - f'(\eta)\} \right] \quad (G.21)$$

The first approximation to the dimensionless temperature in a hypersonic boundary layer with chemical reaction is obtained upon setting  $N = 1$  in equation G.18 and carrying out the indicated integrations. The corresponding integrand for the first integral is obtained from equations G.7, G.16, and G.21.

$$Q(\eta) \equiv Q^{(0)}(\eta, x) = \left( \frac{\sigma c_4}{16 \bar{c}_1 c_3 x} \right) f''(\eta) + 4 \left[ 1 - 2c_2 z^{(0)}(\eta) \right]^{1-m^*} \cdot \left. \begin{aligned} & \prod_{j=1}^{m^*} \left\{ K_j^{(0)} \left[ 1 - \left( \frac{K_p^{(0)}}{K_{pe}^{(0)}} \right)^{m^*} \prod_{j=1}^{m^*} \left( \frac{K_{je}^{(0)}}{K_j^{(0)}} \right) \right. \right. \\ & \left. \left. \exp \left[ \frac{-\beta_1}{1 - 2c_2 z^{(0)}(\eta)} \right] \right] \right\} \right] \quad (G.22)$$

The equilibrium values of the specie weight fractions must be calculated using the zeroth order temperature, equation G.21, and the appropriate value of the pressure.

Higher order solutions may be obtained by continuing the iteration. The integrations will have to be performed numerically; the use of a high speed computing machine would greatly facilitate the numerical calculations.

TABLE I.  
THE BLASIUS FUNCTION AND ITS FIRST THREE  
DERIVATIVES\*

(Flat Plate With No Blowing or Suction)

$\eta$	$f$	$f'$	$f''$	$f'''$
0.00000	0.00000	0.00000	1.32823	0.00000
0.10000	0.00664	0.13282	1.32794	-0.00882
0.20000	0.02656	0.26553	1.32588	-0.03522
0.30000	0.05974	0.39788	1.32032	-0.07887
0.40000	0.10611	0.52942	1.30956	-0.13896
0.50000	0.16557	0.65956	1.29203	-0.21393
0.60000	0.23795	0.78755	1.26636	-0.30133
0.70000	0.32298	0.91252	1.23146	-0.39774
0.80000	0.42032	1.03352	1.18666	-0.49878
0.90000	0.52952	1.14952	1.13173	-0.59927
1.00000	0.65003	1.25953	1.06701	-0.69358
1.10000	0.78120	1.36262	0.99341	-0.77604
1.20000	0.92229	1.45797	0.91237	-0.84147
1.30000	1.07251	1.54491	0.82582	-0.88570
1.40000	1.23098	1.62302	0.73603	-0.90604
1.50000	1.39681	1.69209	0.64544	-0.90156
1.60000	1.56910	1.75216	0.55651	-0.87322
1.70000	1.74695	1.80352	0.47151	-0.82370
1.80000	1.92953	1.84666	0.39235	-0.75705
1.90000	2.11603	1.88224	0.32051	-0.67820
2.00000	2.30575	1.91104	0.25694	-0.59244
2.10000	2.49804	1.93391	0.20208	-0.50481
2.20000	2.69237	1.95174	0.15590	-0.41973
2.30000	2.88825	1.96537	0.11794	-0.34064
2.40000	3.08533	1.97558	0.08749	-0.26994
2.50000	3.28328	1.98308	0.06363	-0.20893
2.60000	3.48187	1.98849	0.04537	-0.15799
2.70000	3.68093	1.99231	0.03172	-0.11675
2.80000	3.88030	1.99496	0.02173	-0.08434
2.90000	4.07989	1.99675	0.01460	-0.05957

\* Reference 70.

TABLE I. Continued

$\eta$	$f$	$f'$	$f''$	$f'''$
3.00000	4.27963	1.99795	0.00961	-0.04114
3.10000	4.47946	1.99873	0.00621	-0.02780
3.20000	4.67936	1.99922	0.00393	-0.01837
3.30000	4.87930	1.99954	0.00244	-0.01188
3.40000	5.07927	1.99973	0.00148	-0.00752
3.50000	5.27925	1.99984	0.00088	-0.00466
3.60000	5.47923	1.99991	0.00052	-0.00283
3.70000	5.67923	1.99995	0.00030	-0.00168
3.80000	5.87922	1.99997	0.00017	-0.00098
3.90000	6.07922	1.99999	0.00009	-0.00056
4.00000	6.27922	1.99999	0.00005	-0.00031
4.10000	6.47922	2.00000	0.00003	-0.00017
4.20000	6.67922	2.00000	0.00001	-0.00009
4.30000	6.87922	2.00000	0.00001	-0.00005
4.40000	7.07922	2.00000	0.00000	-0.00002
4.50000	7.27922	2.00000	0.00000	-0.00001
4.60000	7.47922	2.00000	0.00000	-0.00001
4.70000	7.67922	2.00000	0.00000	-0.00000
4.80000	7.87922	2.00000	0.00000	-0.00000
4.90000	8.07922	2.00000	0.00000	-0.00000
5.00000	8.27922	2.00000	0.00000	-0.00000



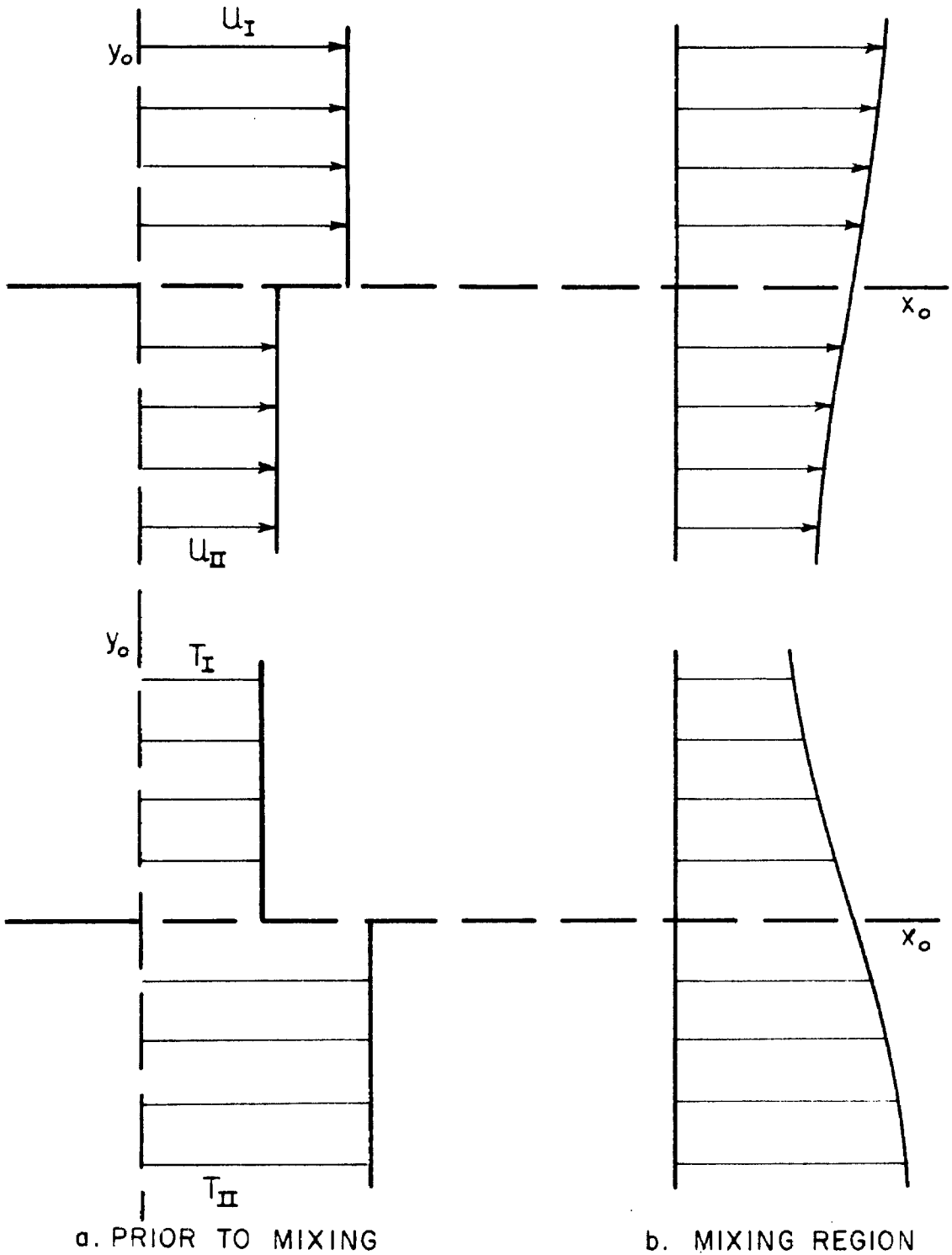


FIGURE 1  
TYPICAL VELOCITY AND TEMPERATURE PROFILES  
FOR A MIXING REGION WITHOUT CHEMICAL REACTION

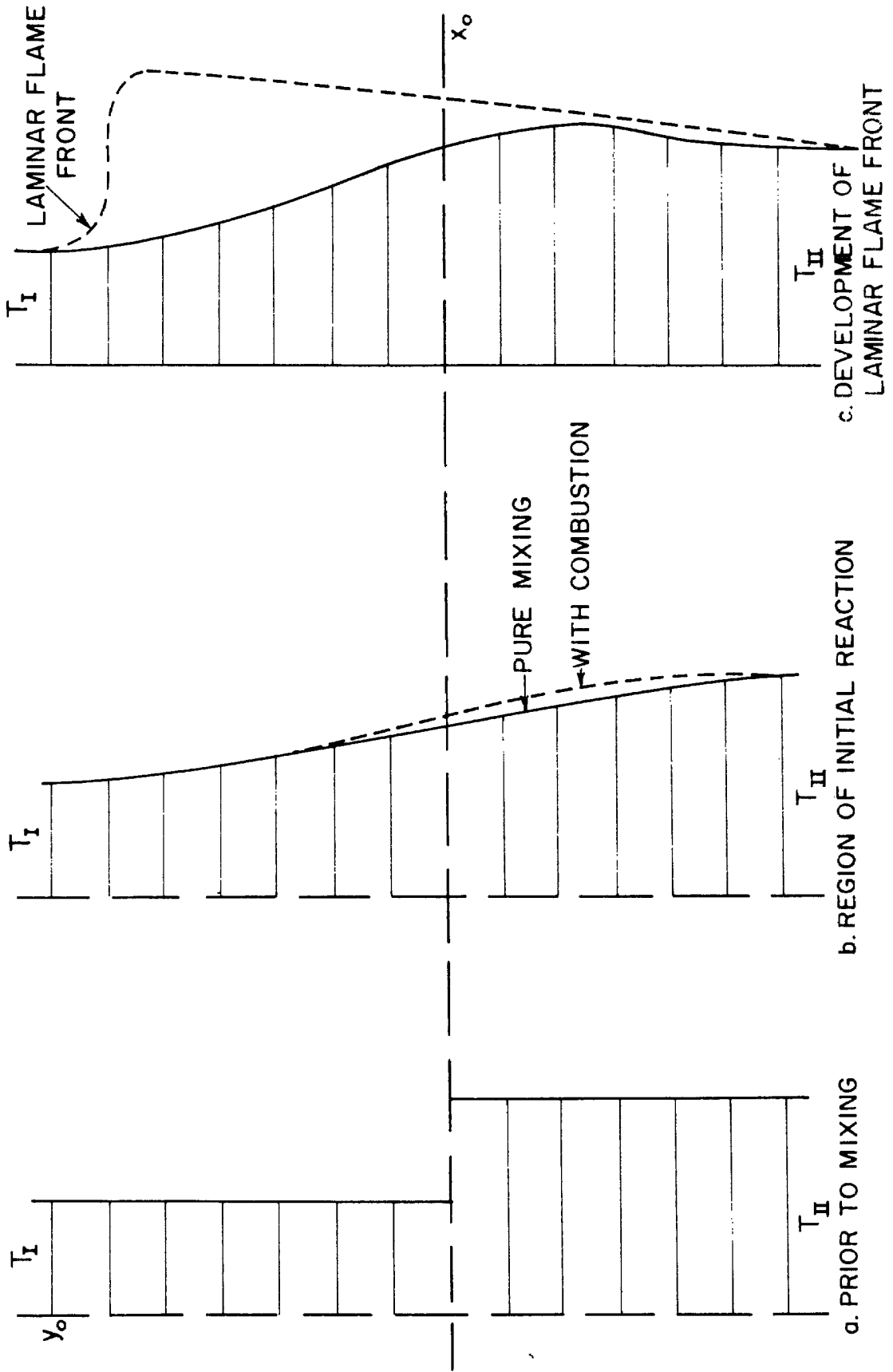


FIGURE 2

TYPICAL TEMPERATURE PROFILES IN A REACTING REGION WITH CHEMICAL REACTION

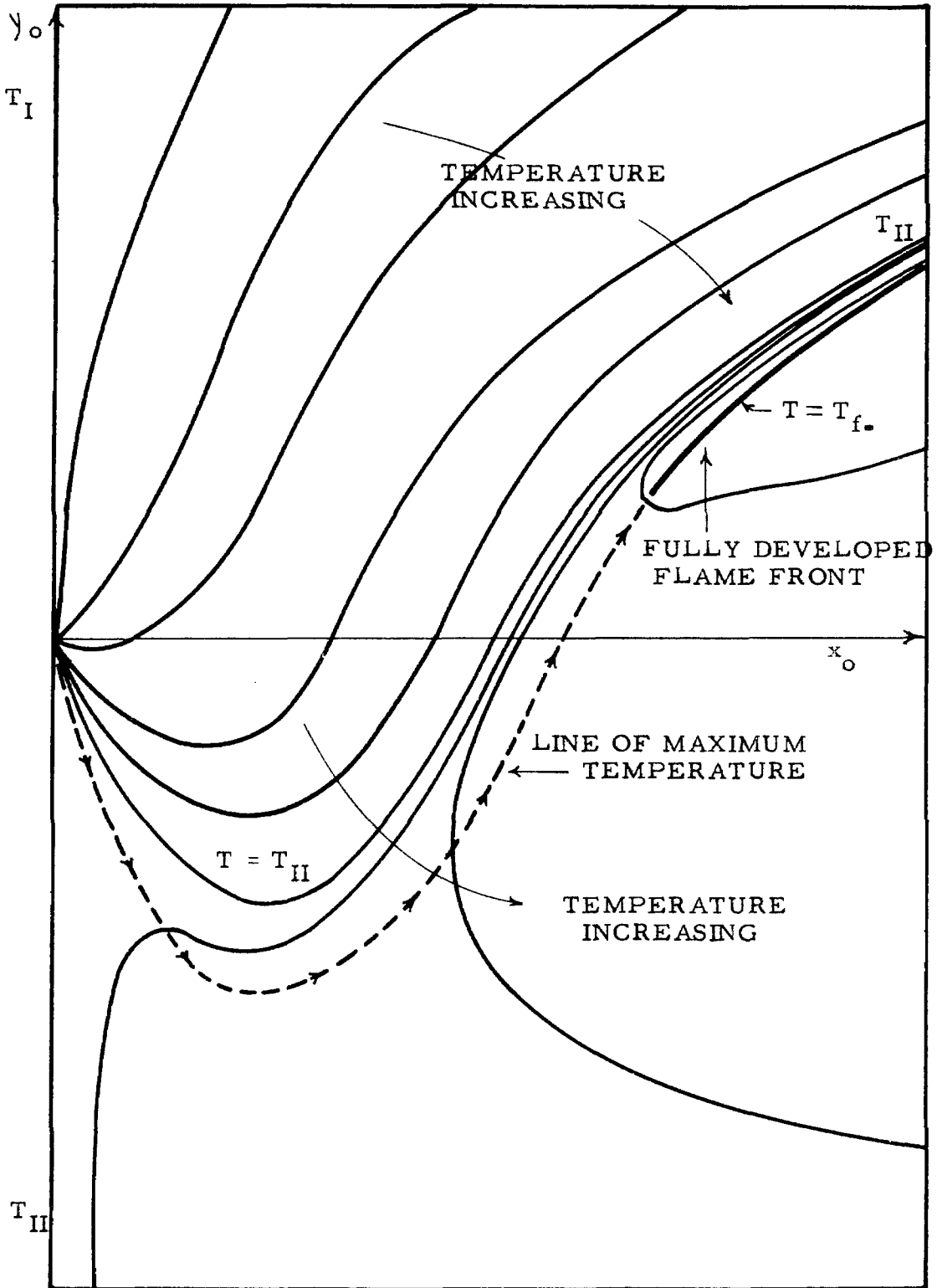
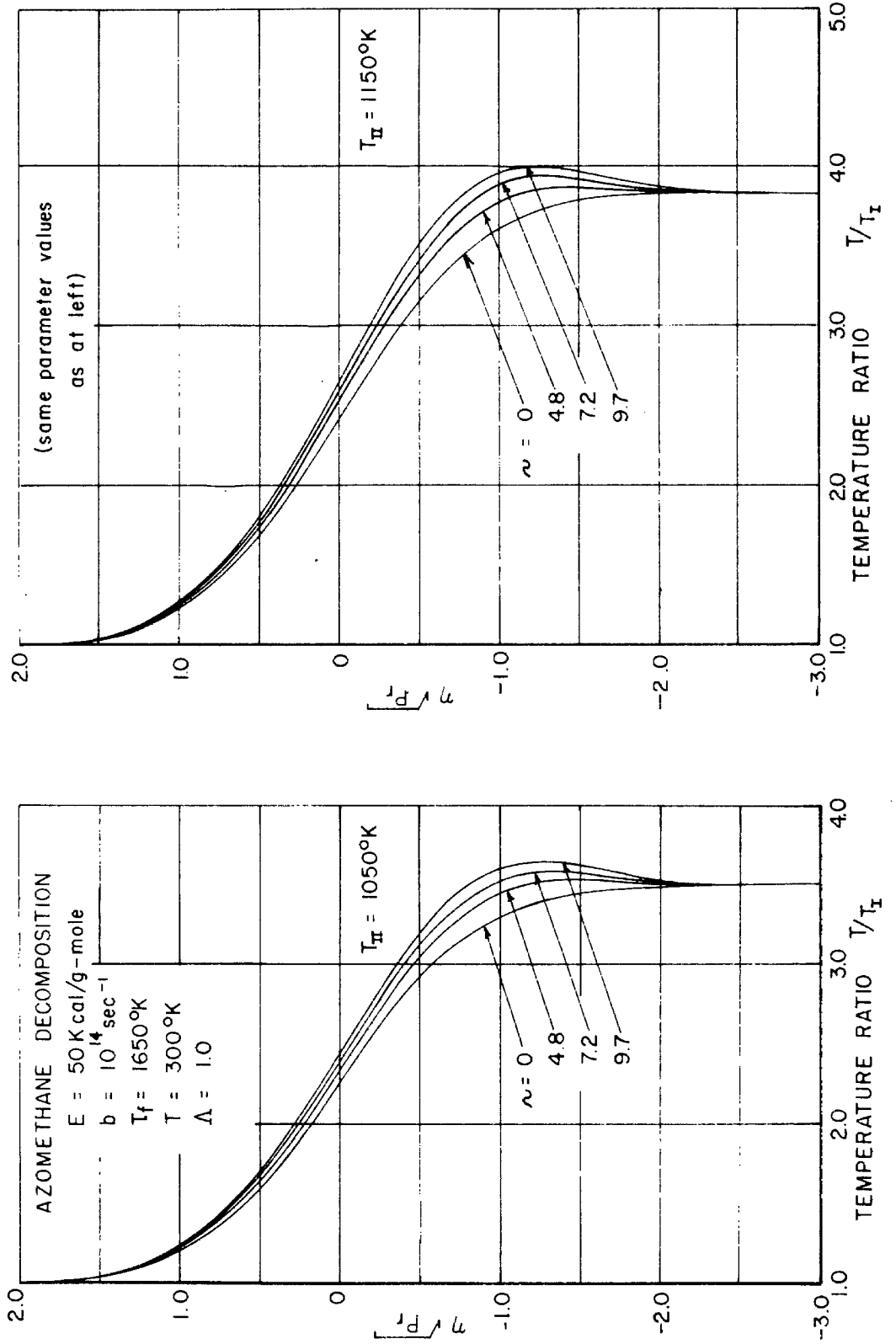


FIGURE 3  
TYPICAL ISOTHERM FIELD FOR A MIXING REGION  
WITH CHEMICAL REACTION

FIGURE 4

TEMPERATURE PROFILES DURING THE EARLY STAGES OF A FIRST-ORDER REACTION IN A SHEAR-FREE MIXING REGION



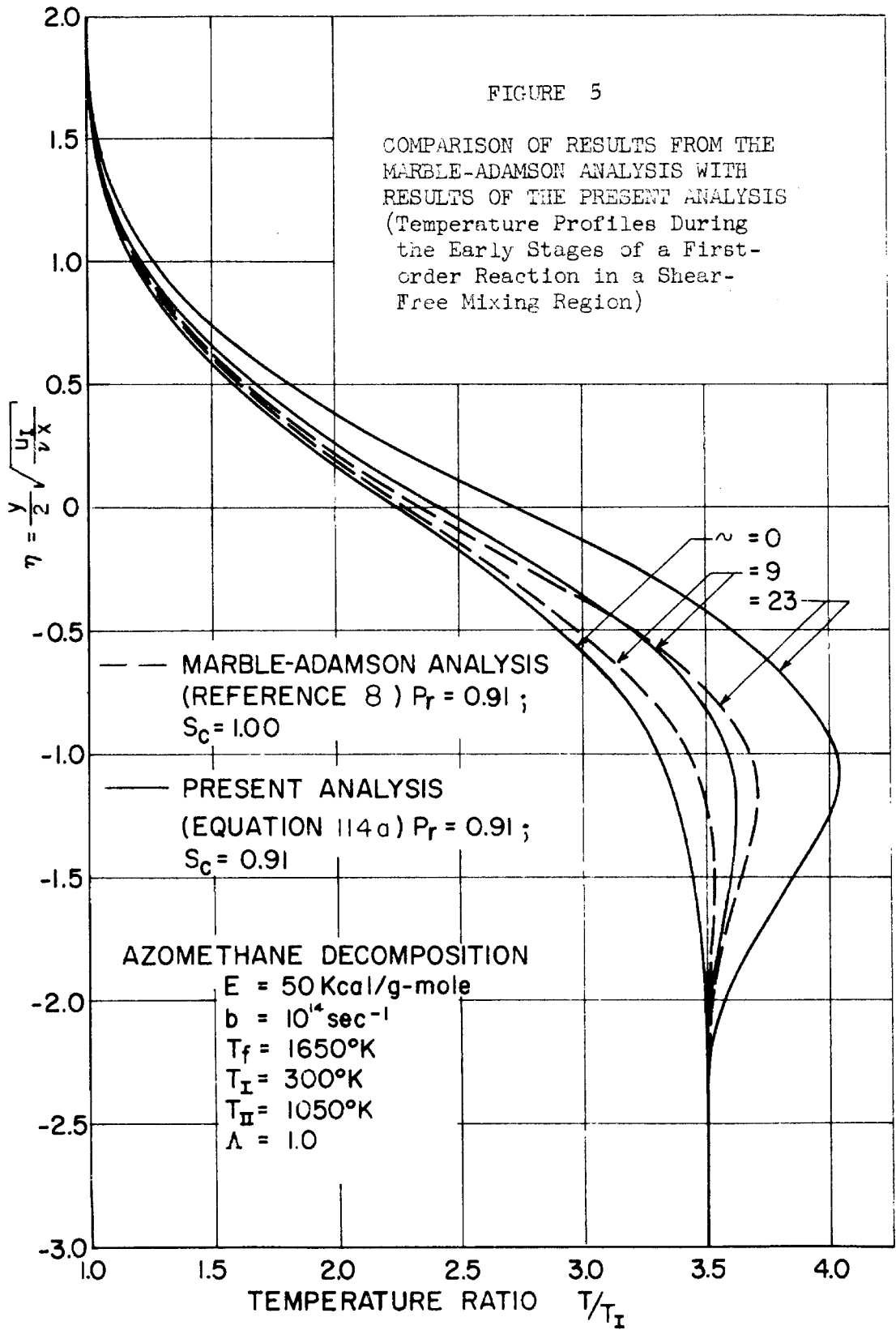
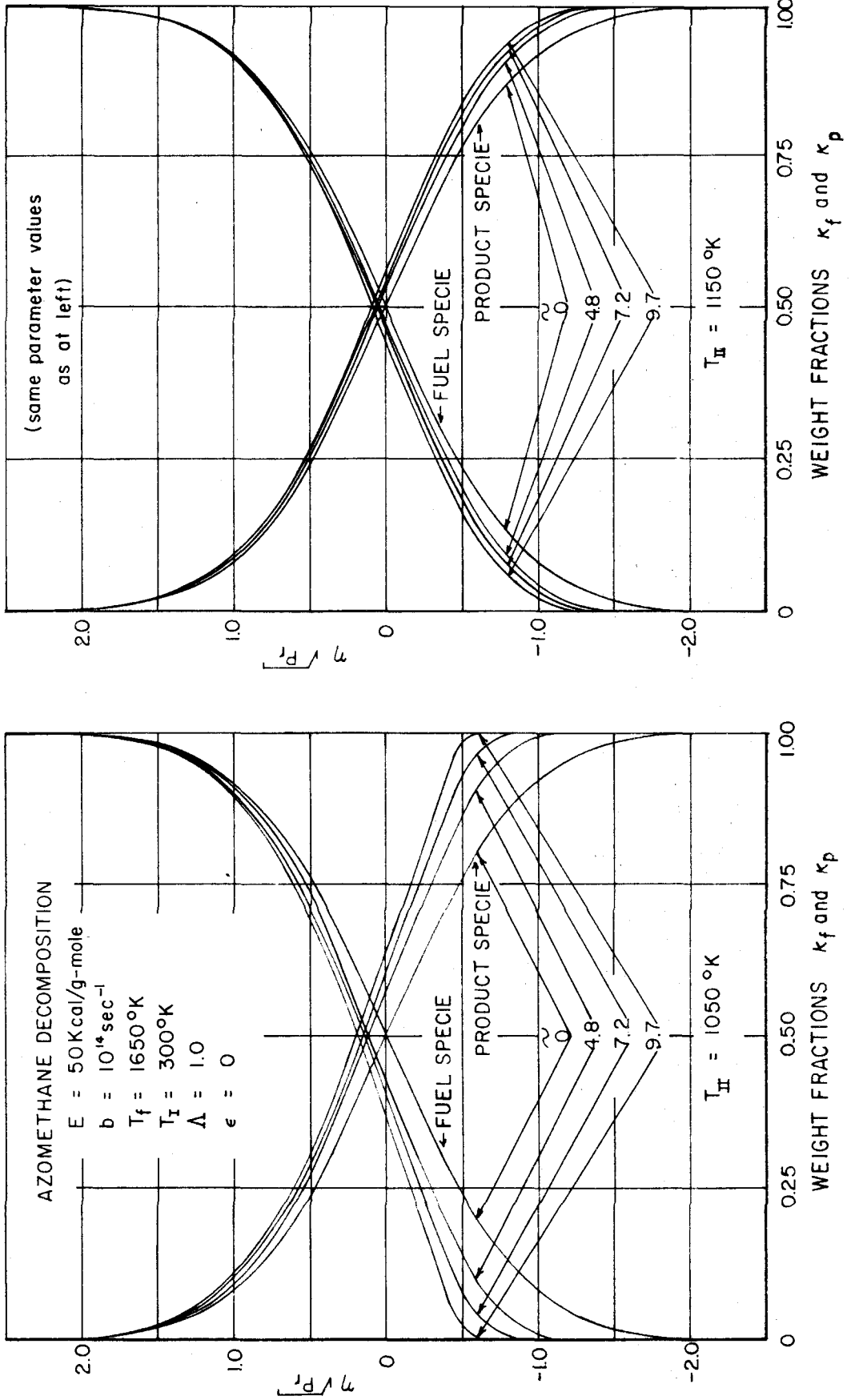
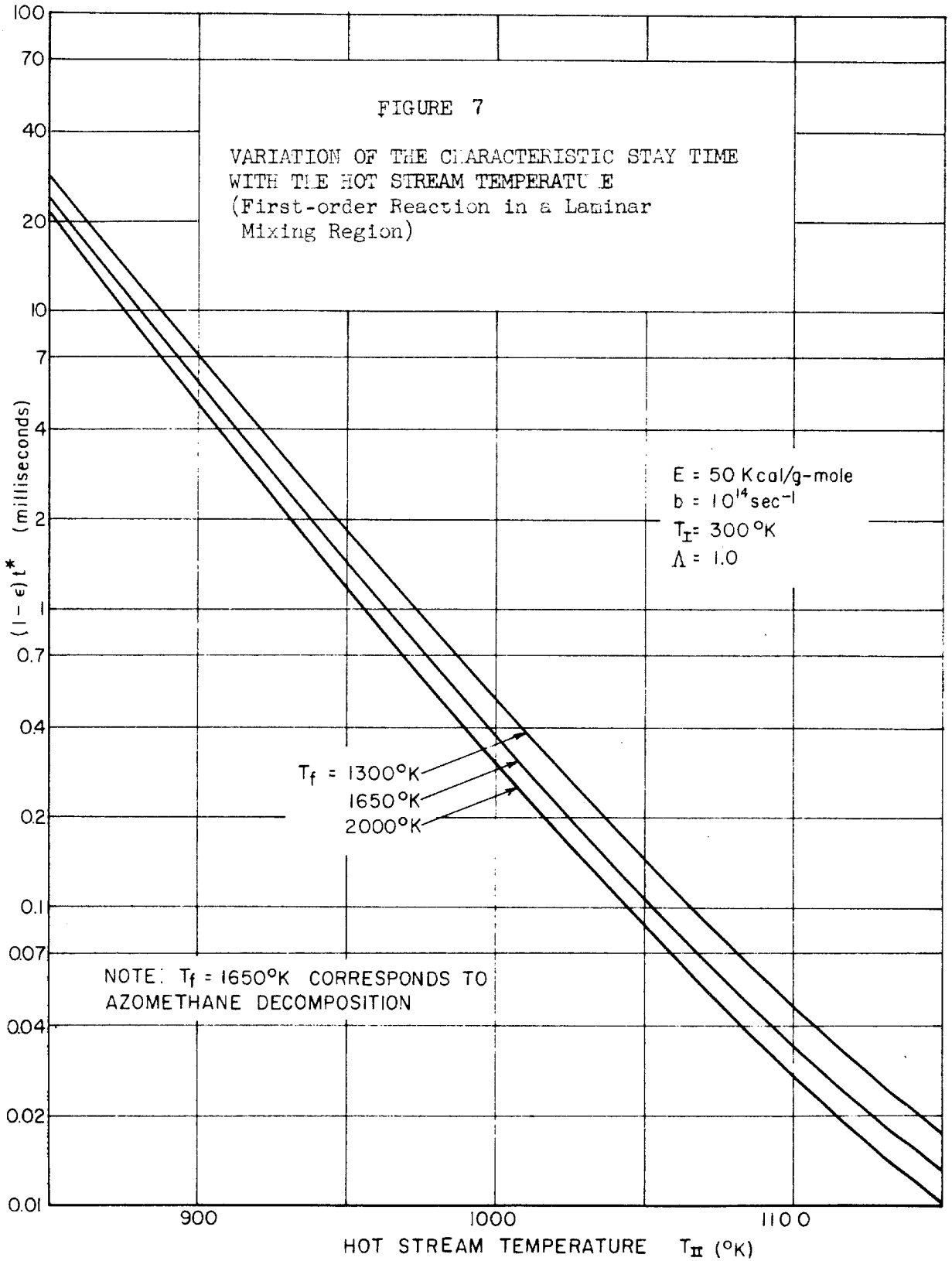
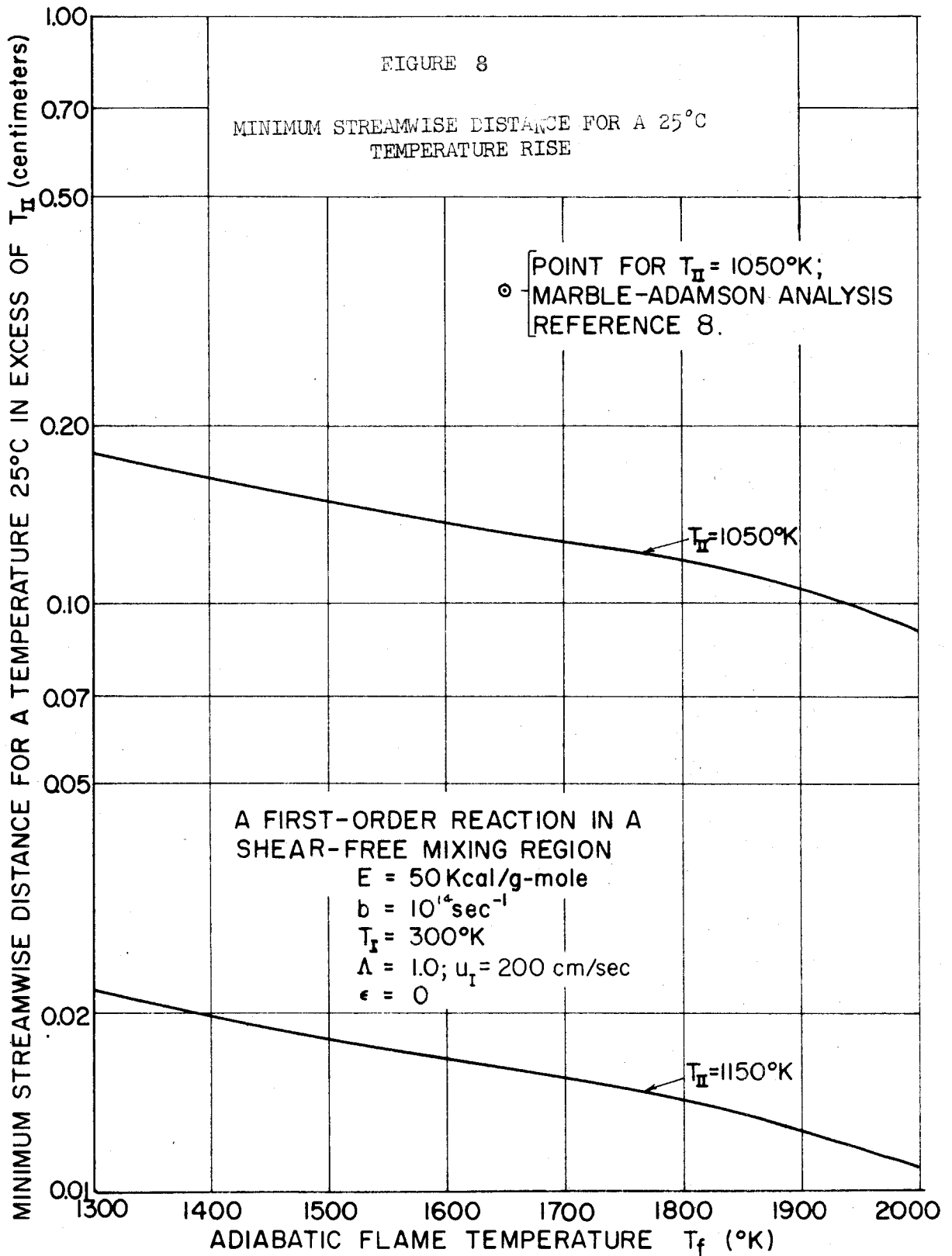


FIGURE 6

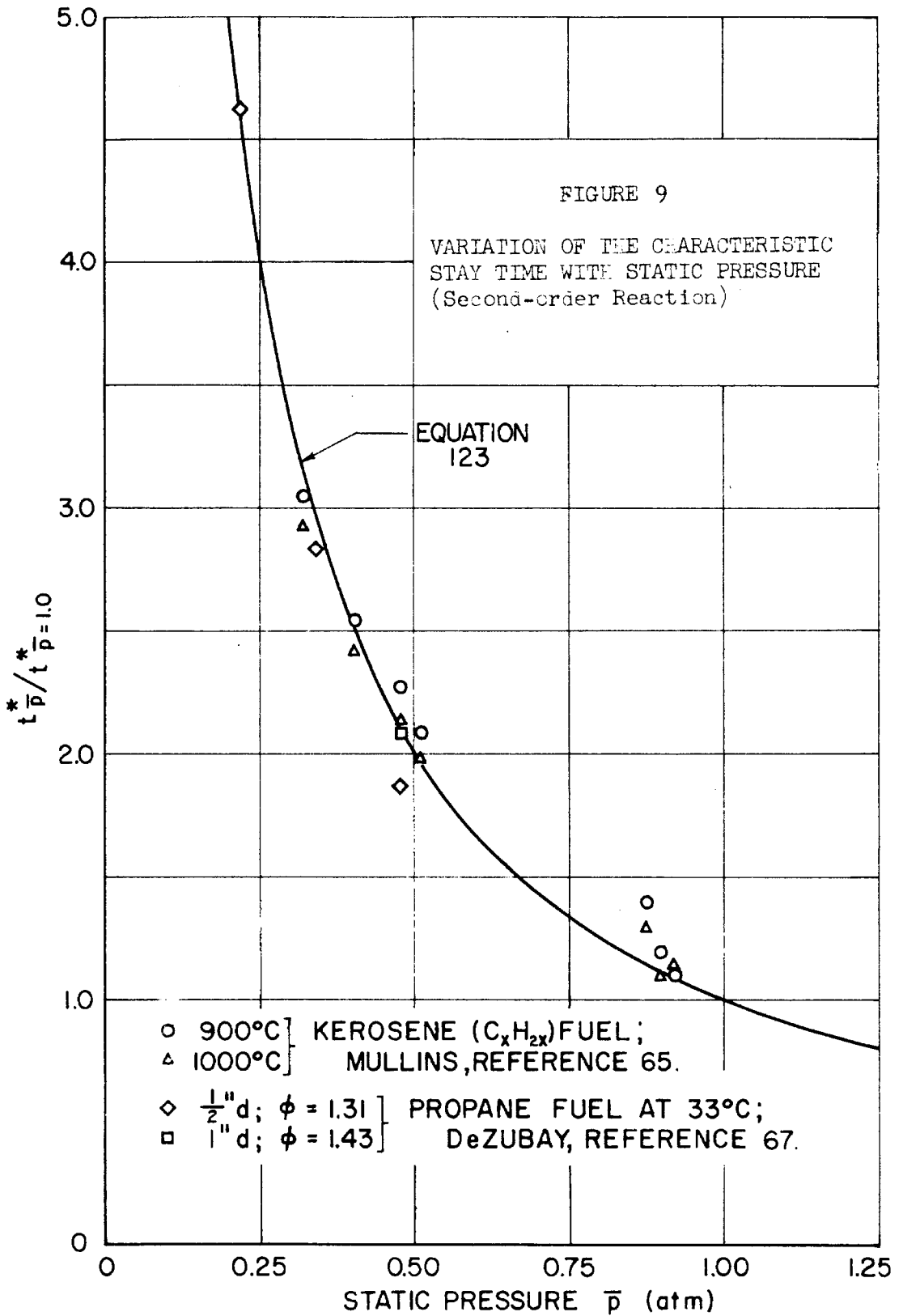
CONCENTRATION PROFILES DURING THE EARLY STAGES OF A FIRST-ORDER REACTION IN A SHEAR-FREE MIXING REGION

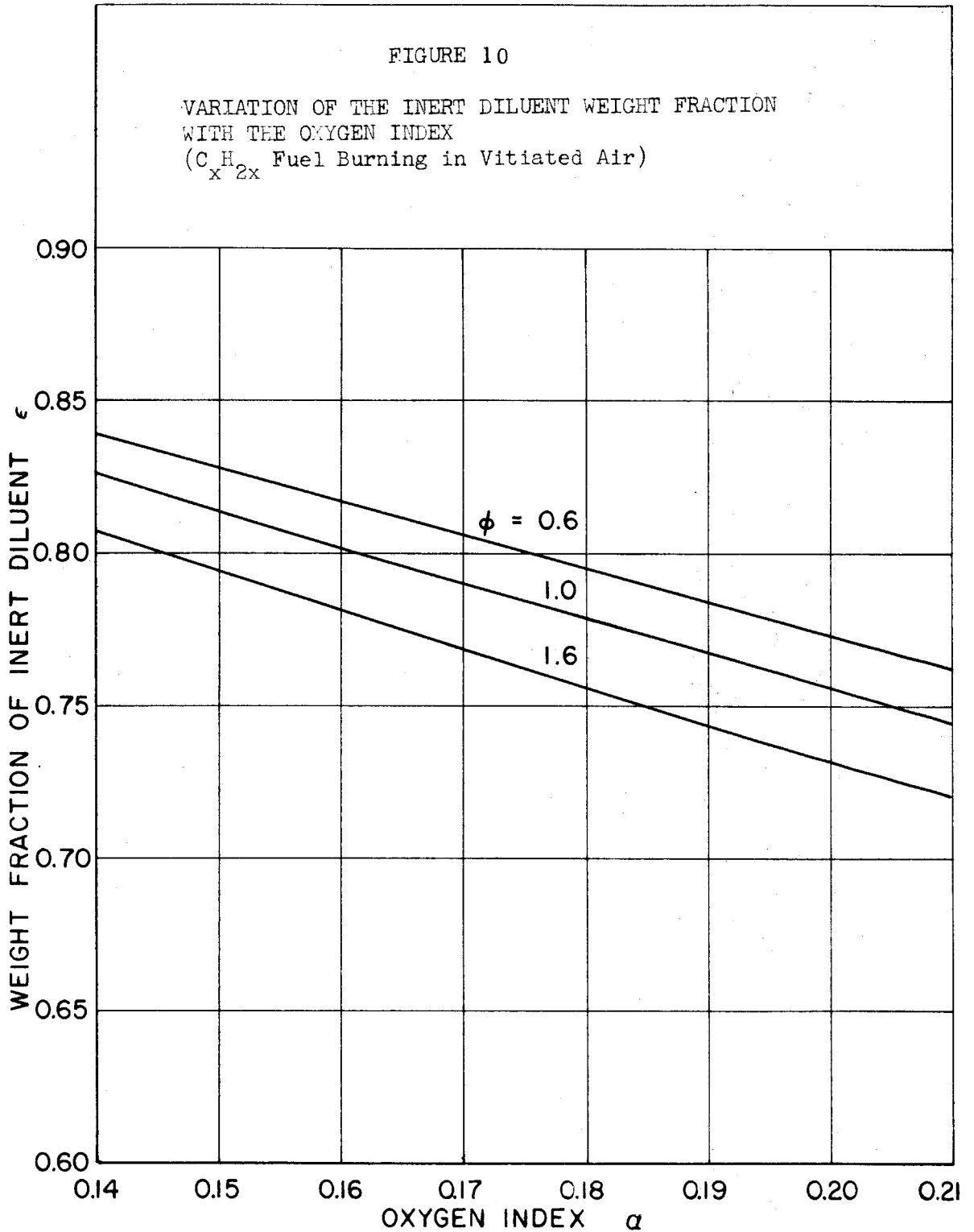


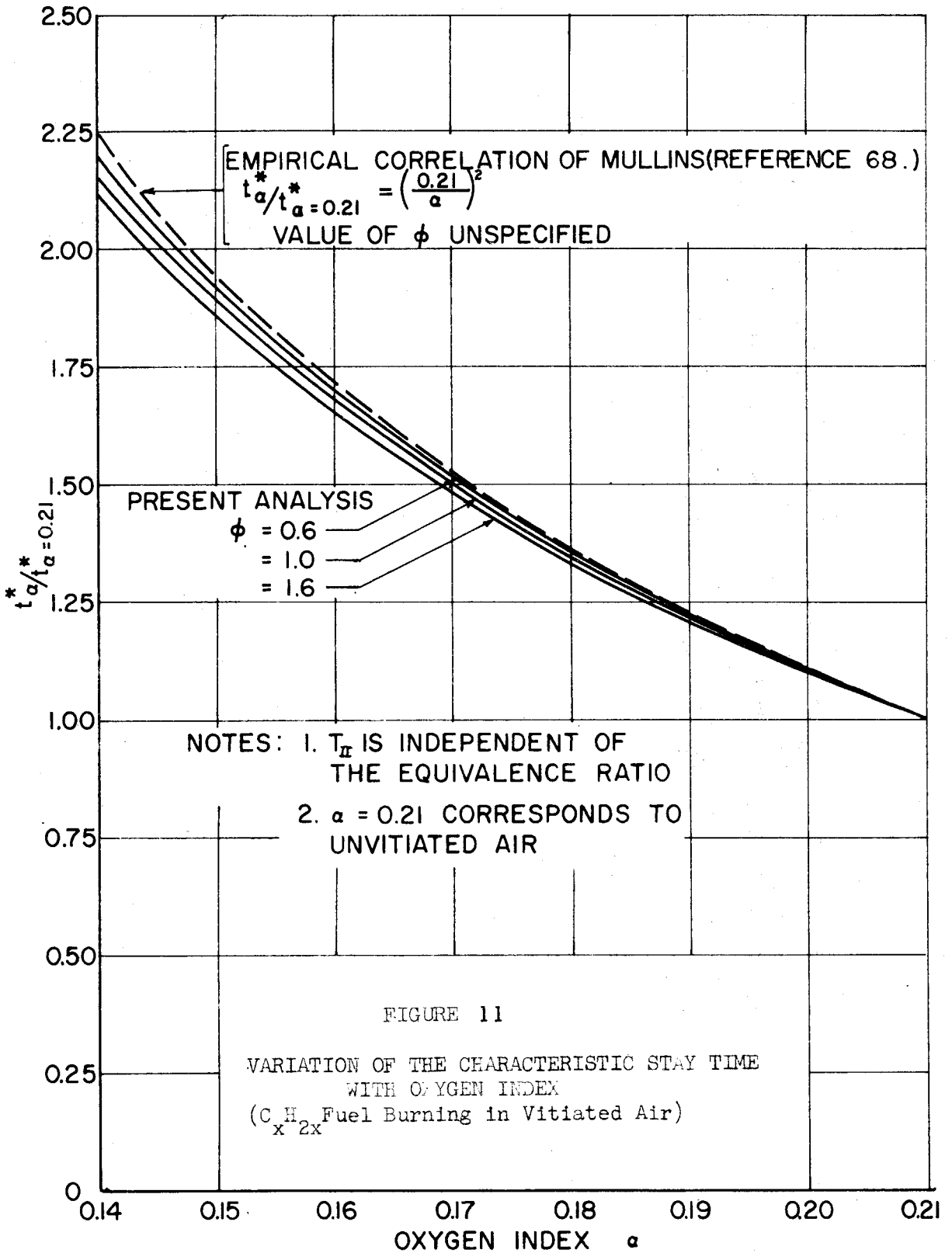


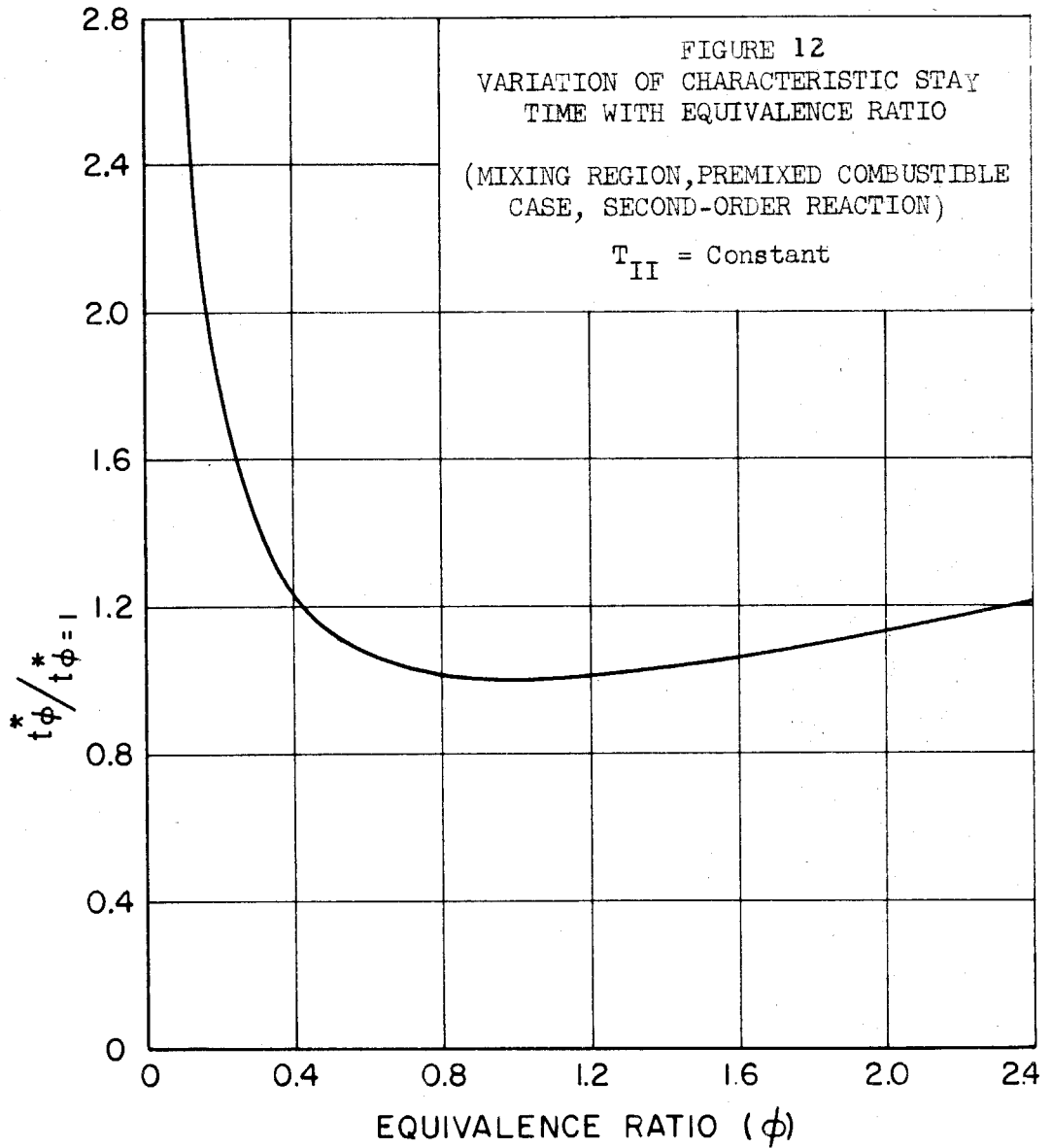












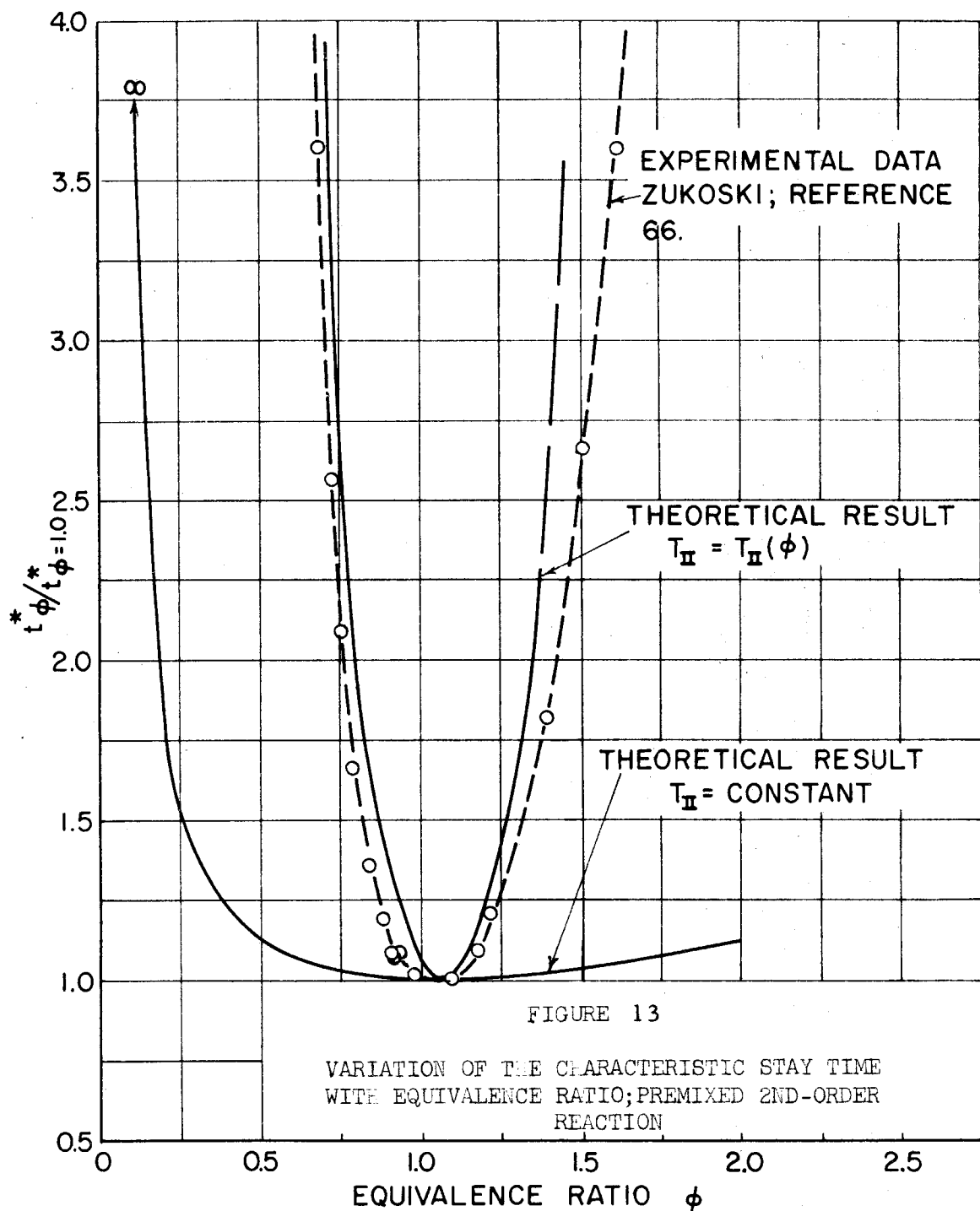
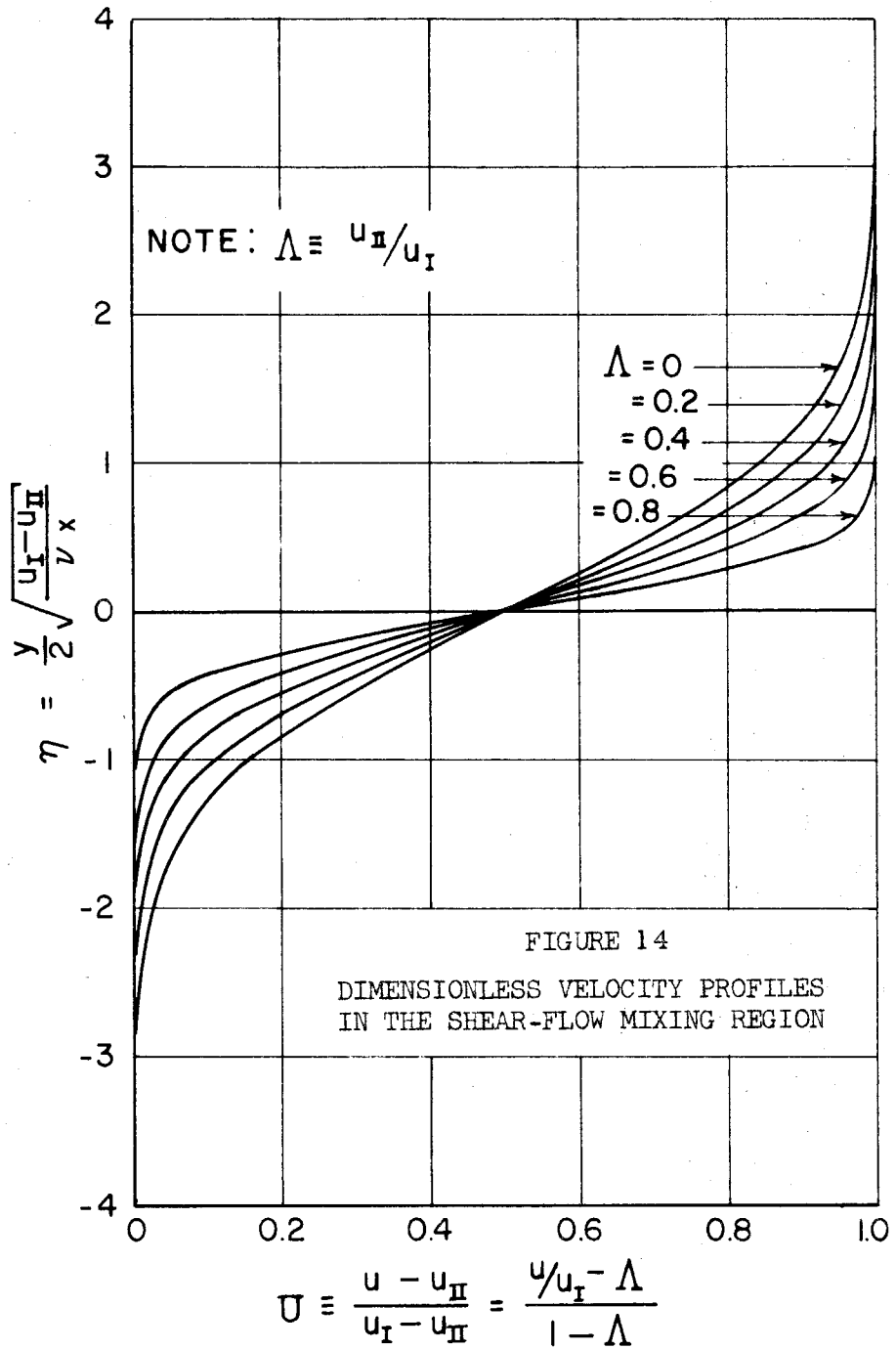
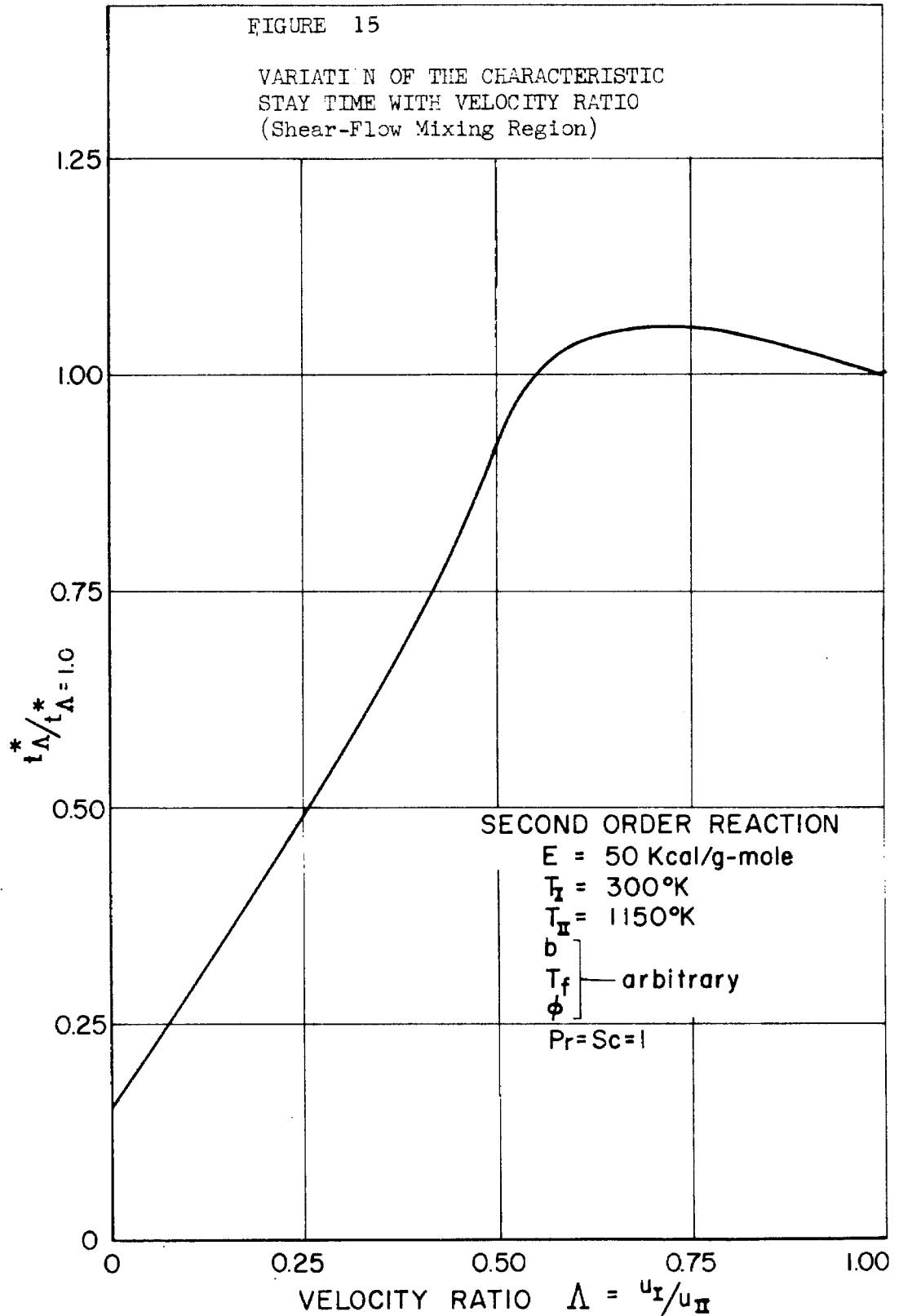
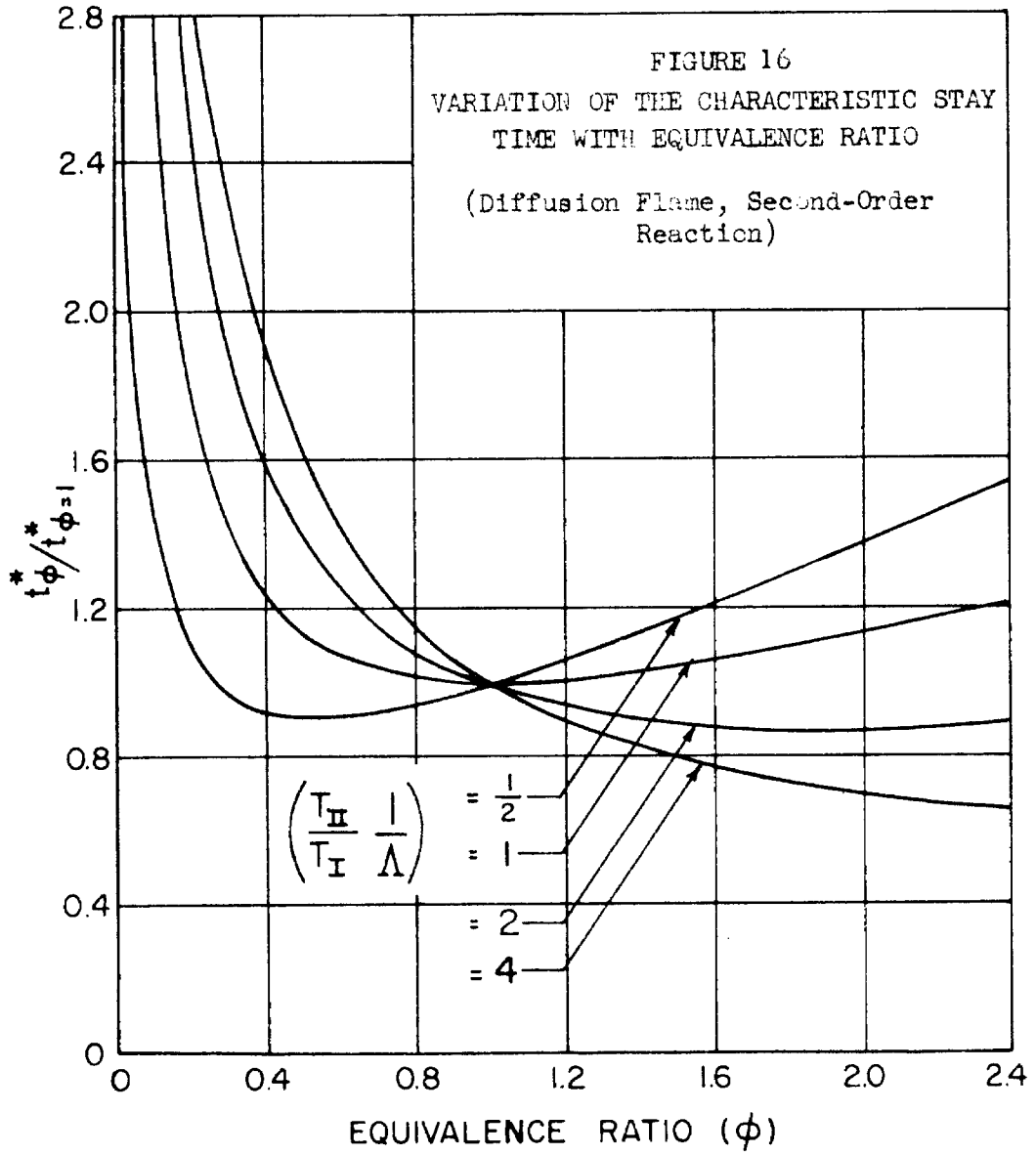


FIGURE 13

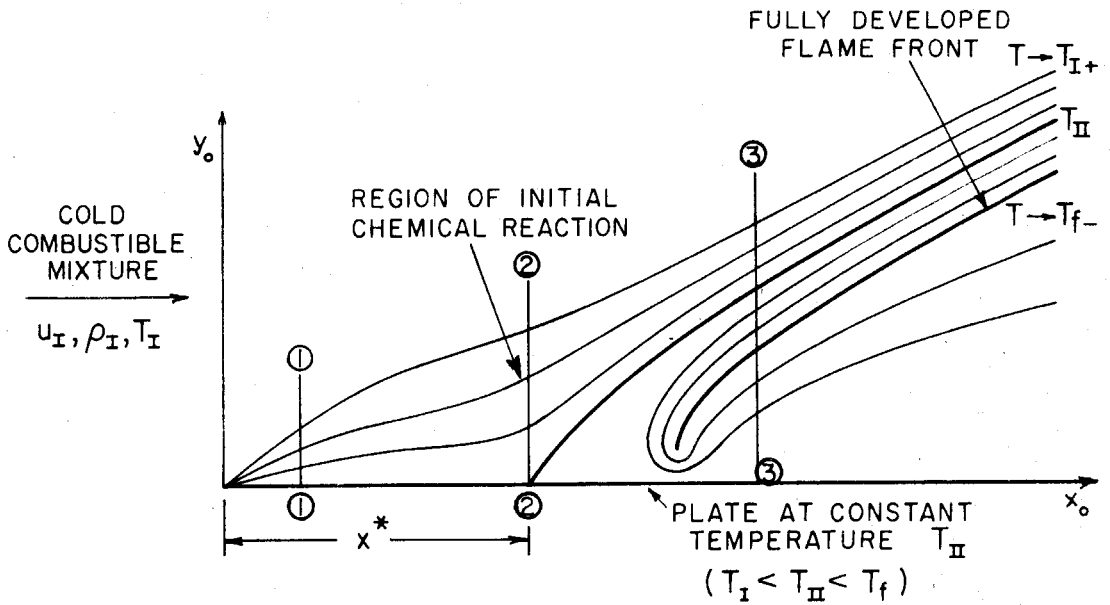
VARIATION OF THE CHARACTERISTIC STAY TIME WITH EQUIVALENCE RATIO; PREMIXED 2ND-ORDER REACTION





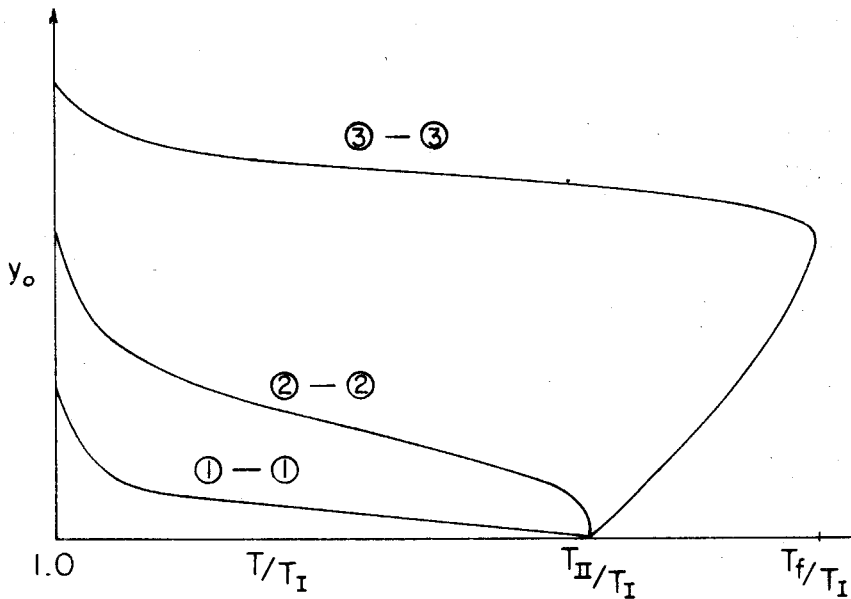






a. TYPICAL ISOTHERM FIELD

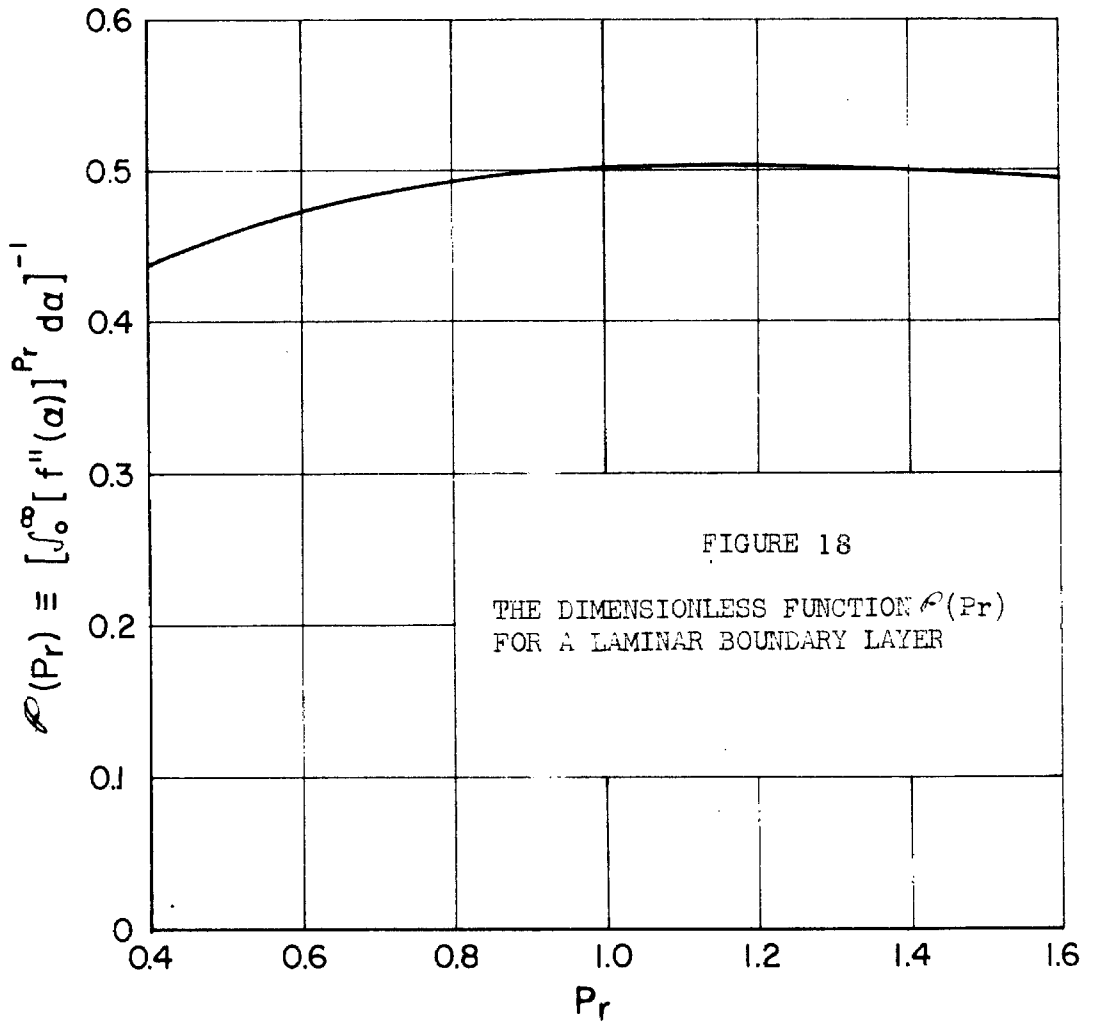
NOTE: VERTICAL SCALES ARE GREATLY ENLARGED

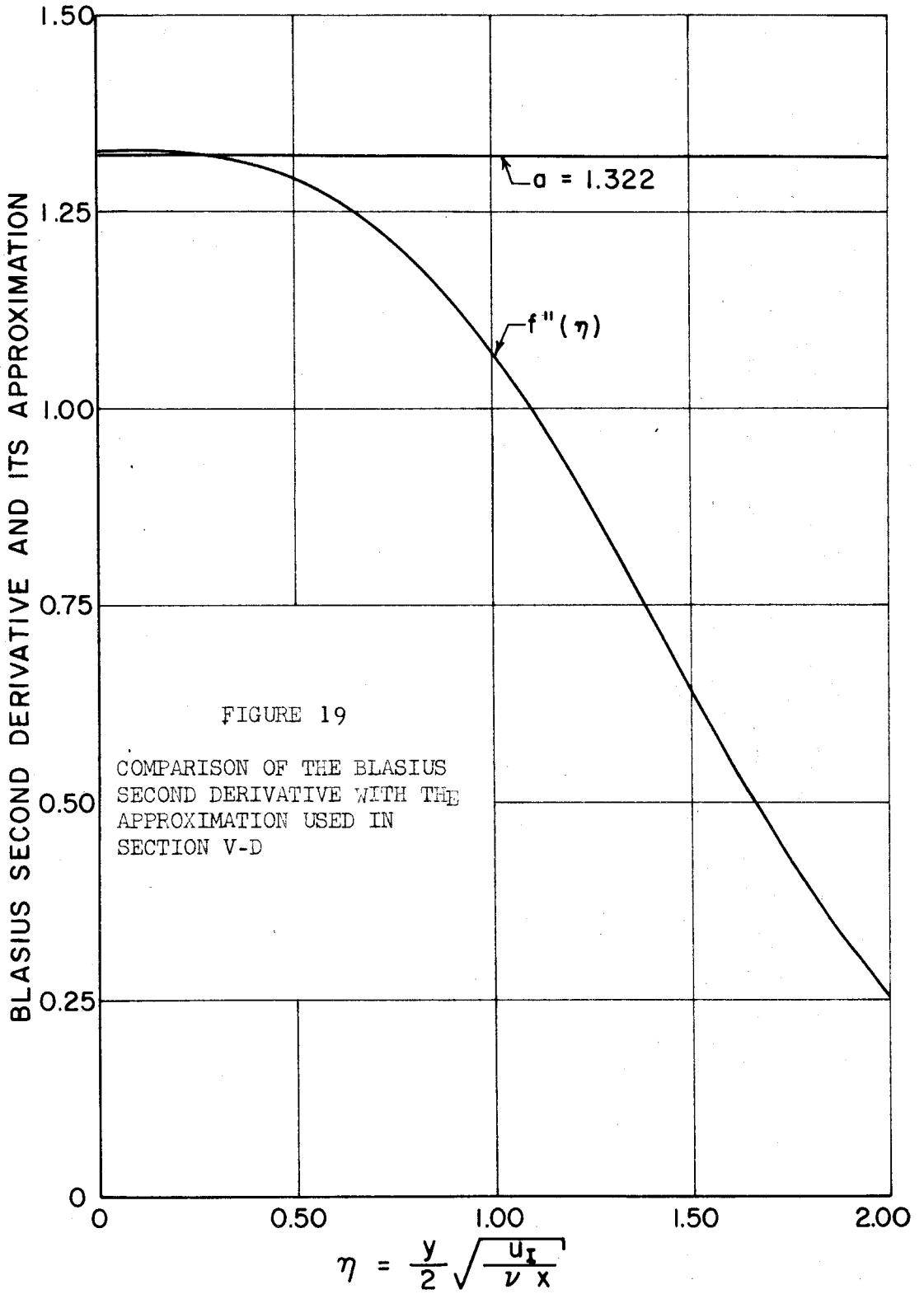


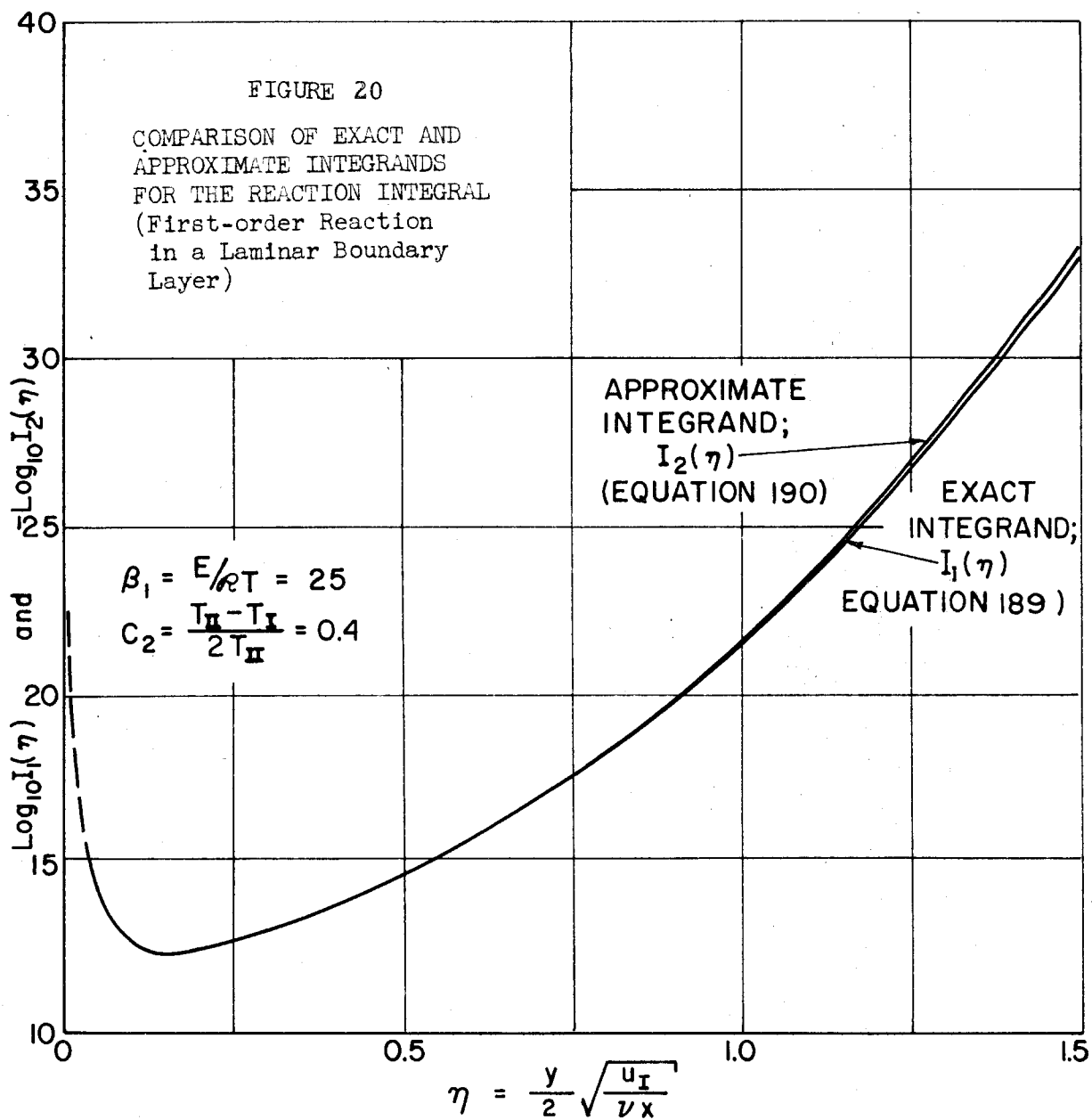
b. TYPICAL TEMPERATURE PROFILES

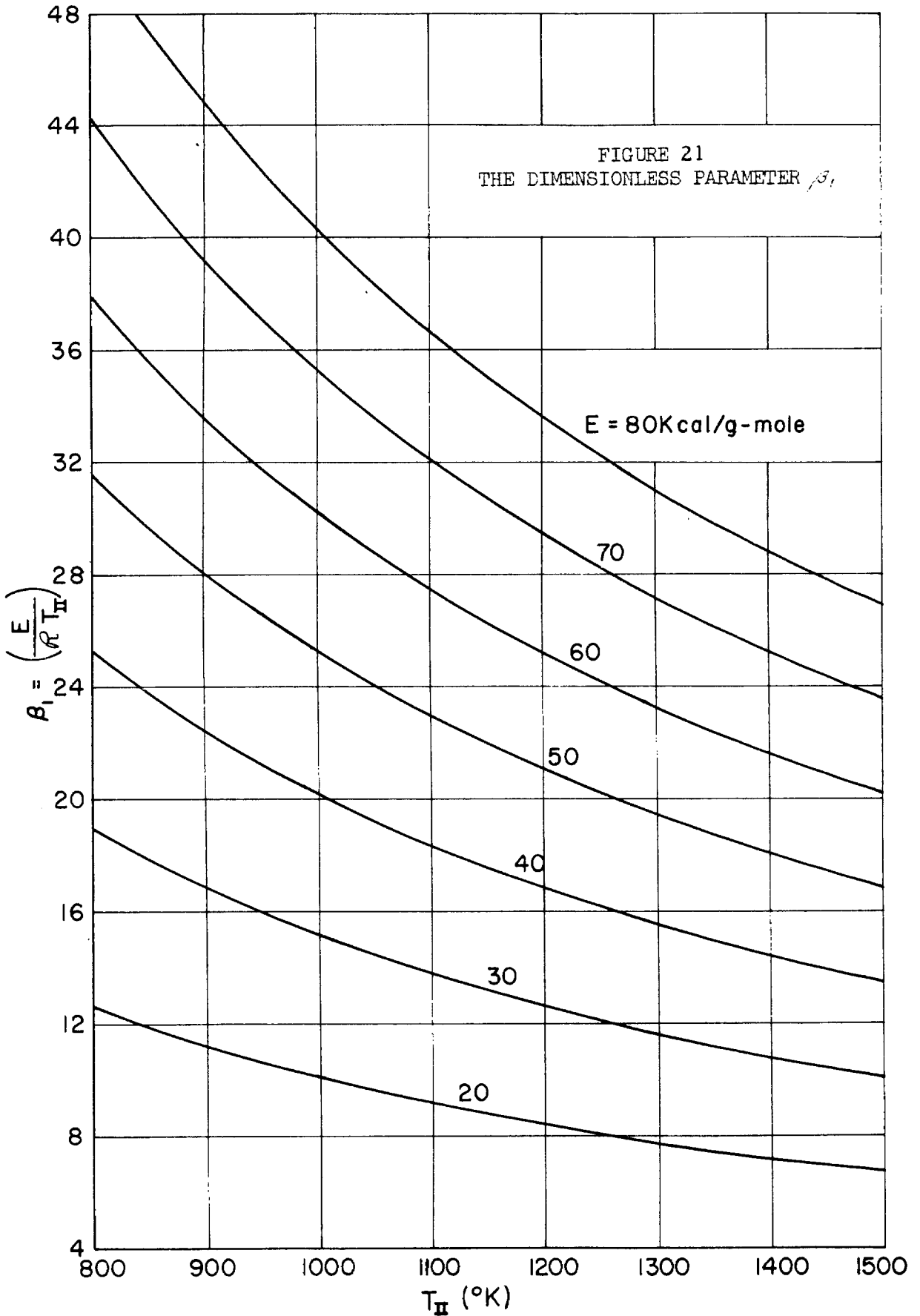
FIGURE 17

COMBUSTION IN THE LAMINAR BOUNDARY LAYER









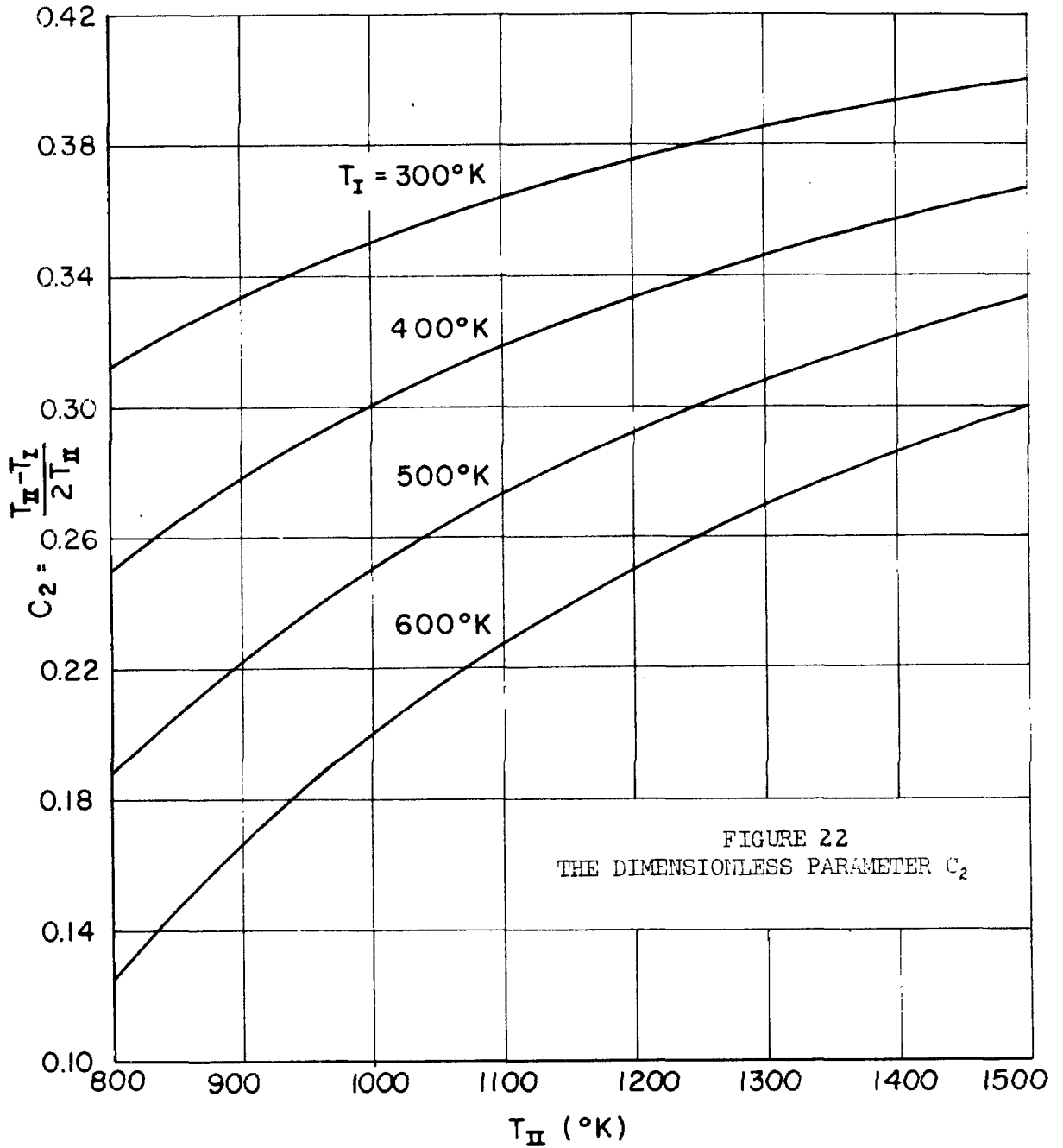


FIGURE 22  
THE DIMENSIONLESS PARAMETER  $C_2$

FIGURE  
THE DIMENSIONLESS PARAMETER  $C_2$

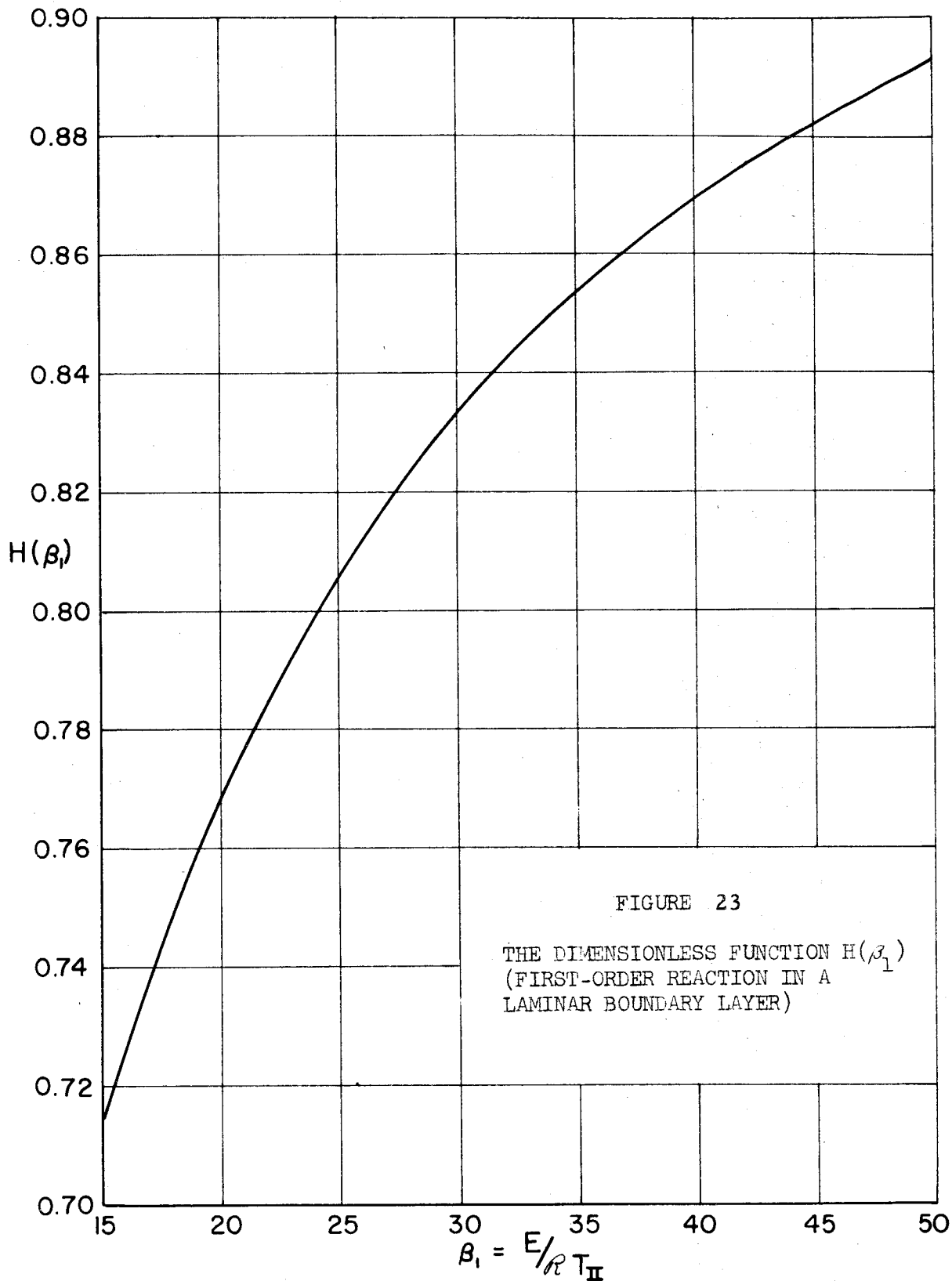
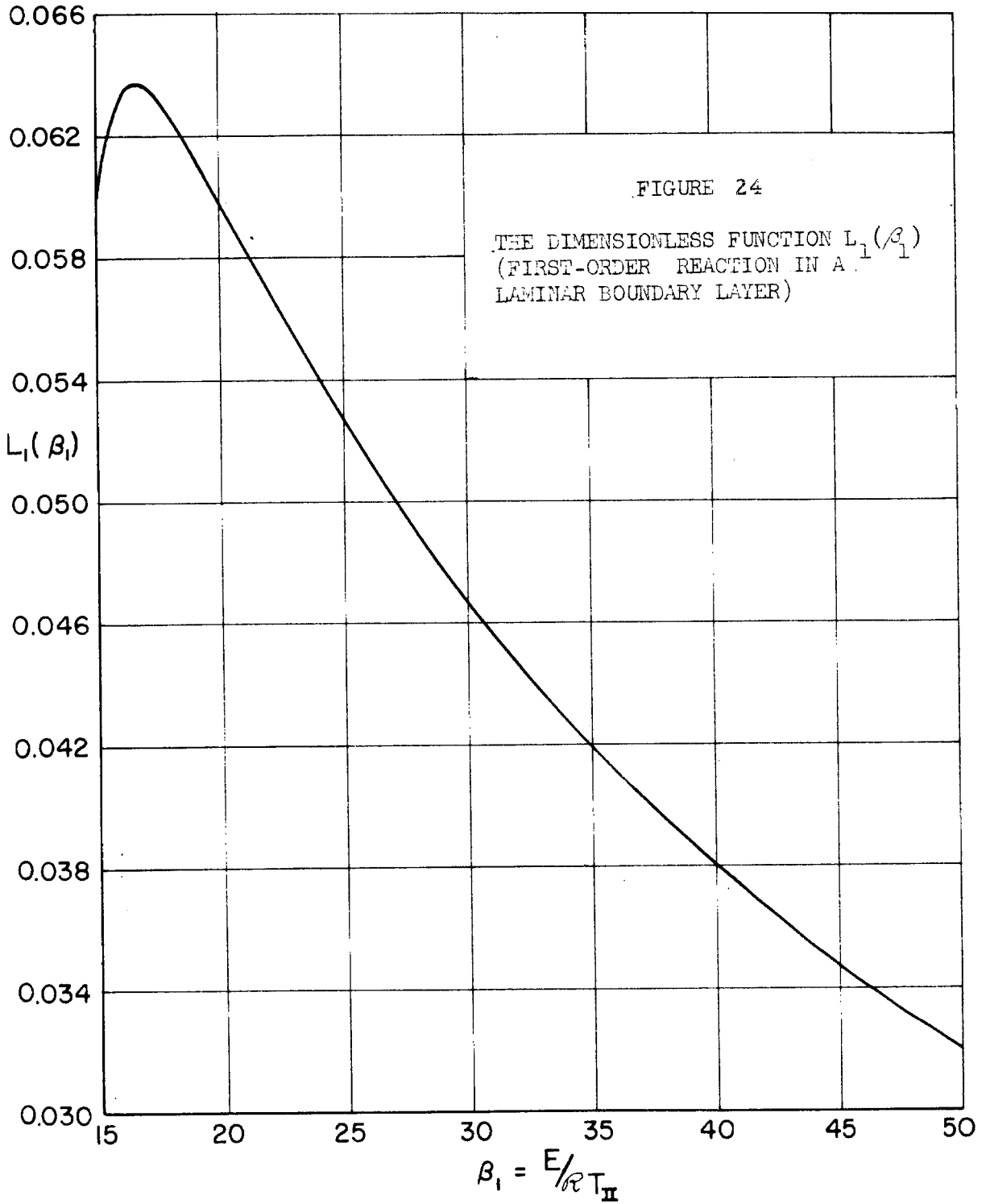


FIGURE 23

THE DIMENSIONLESS FUNCTION  $H(\beta_1)$   
(FIRST-ORDER REACTION IN A  
LAMINAR BOUNDARY LAYER)





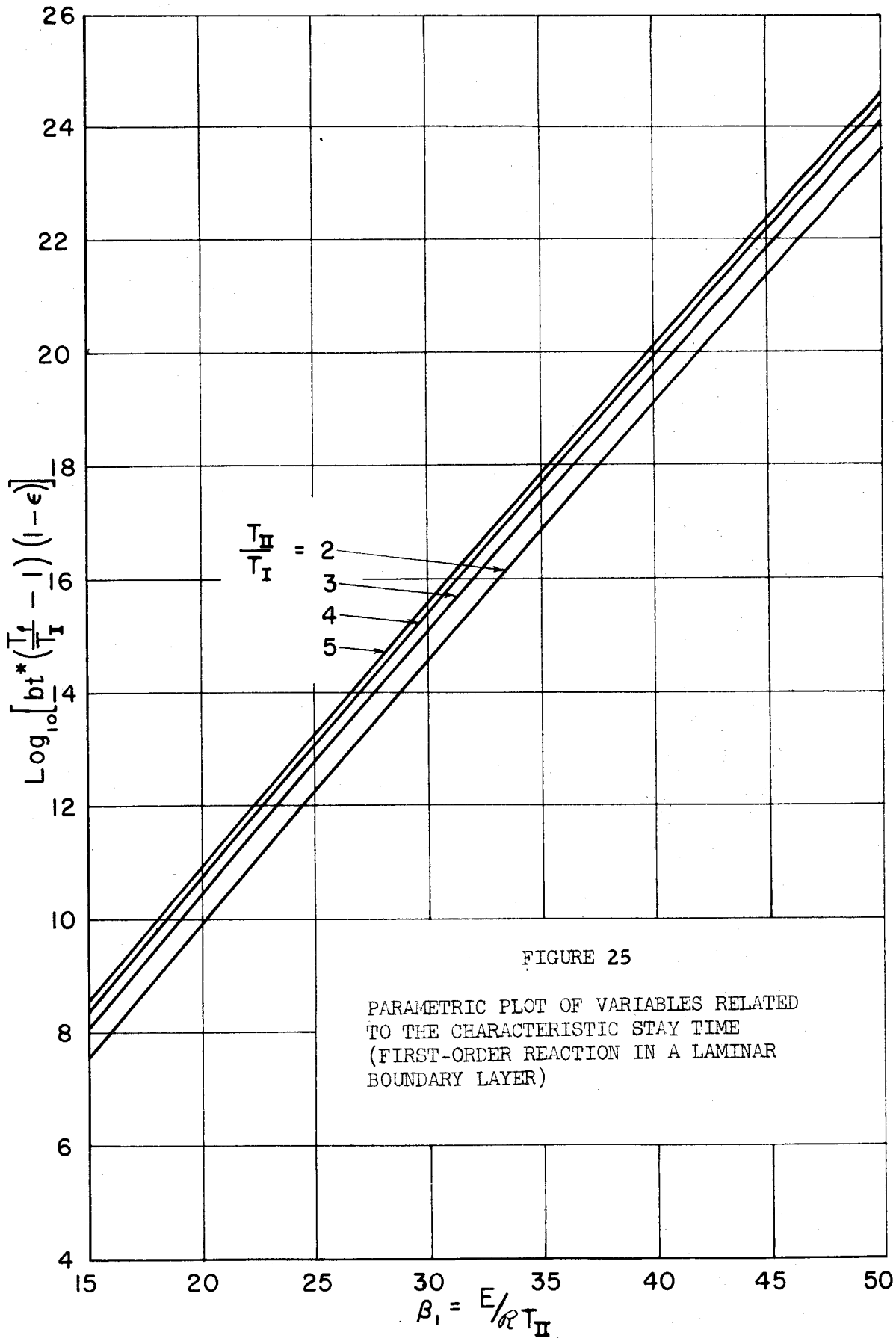
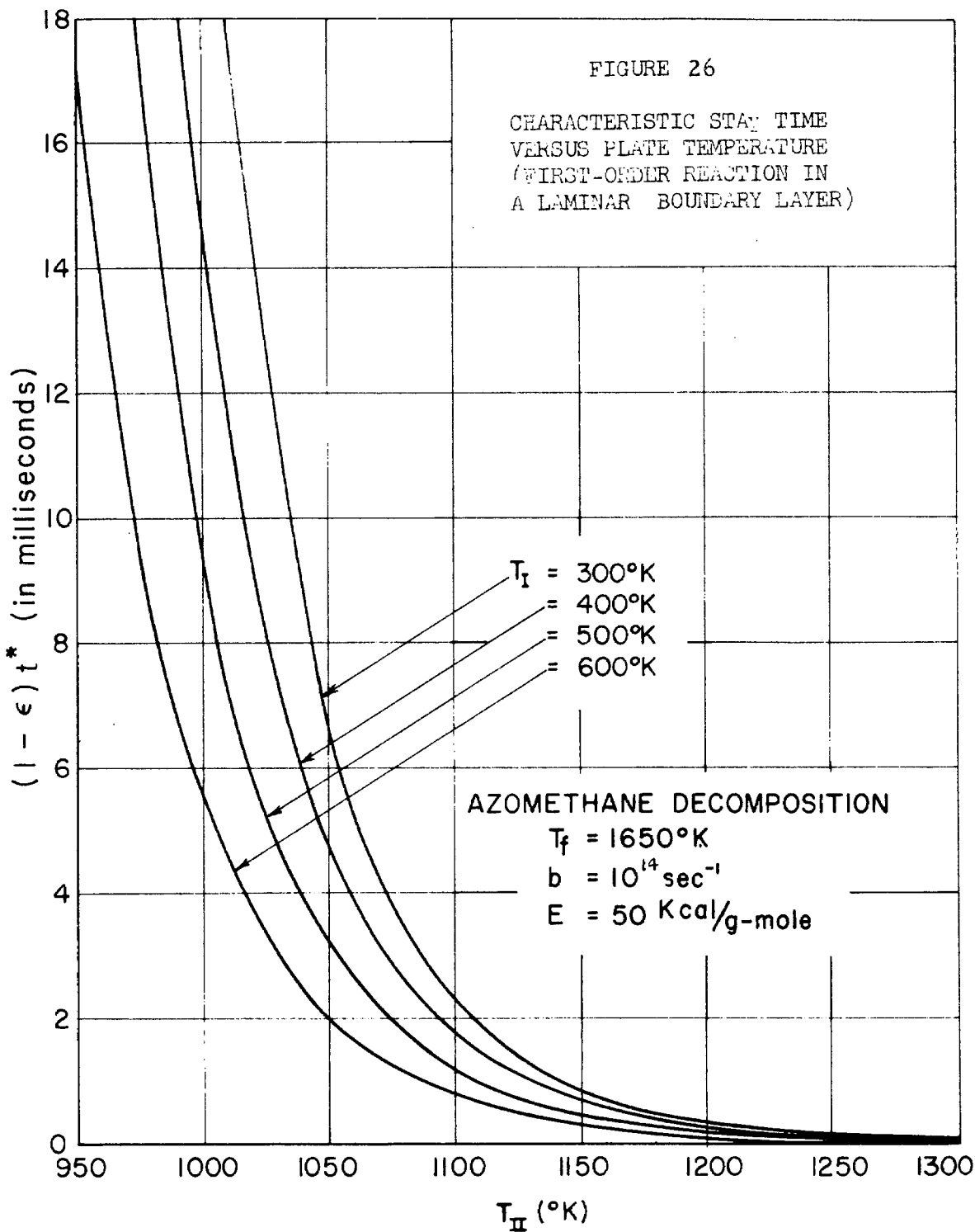
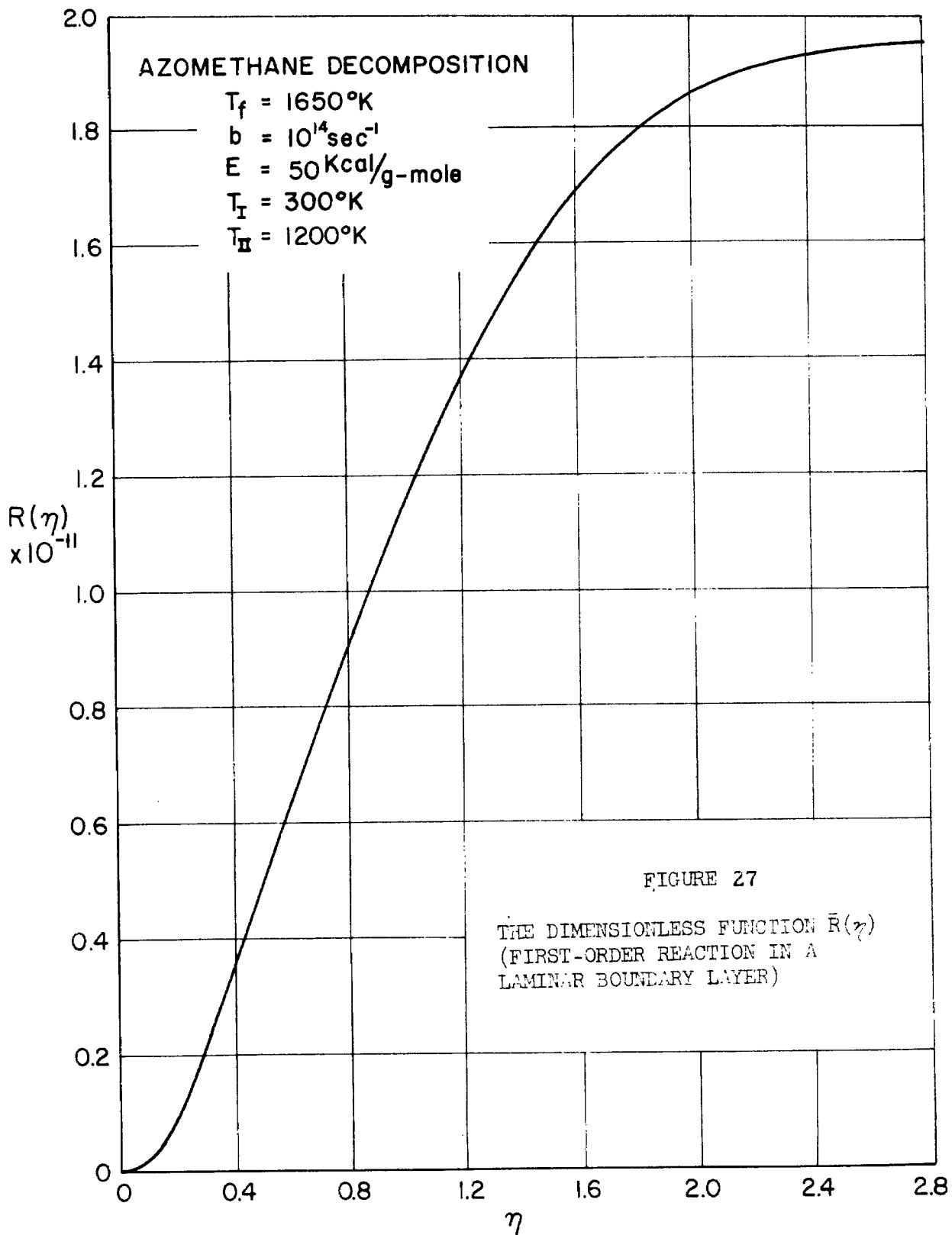
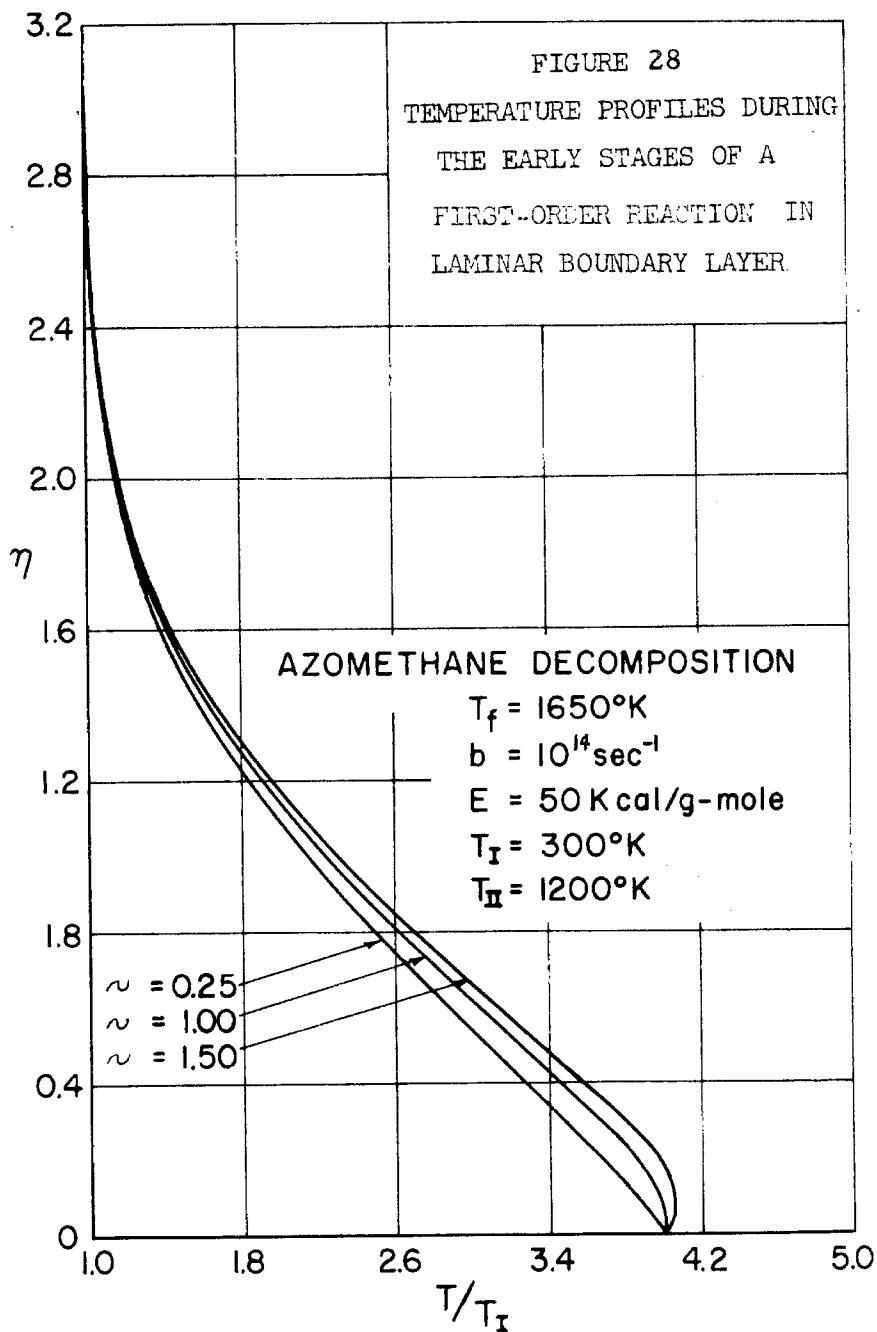


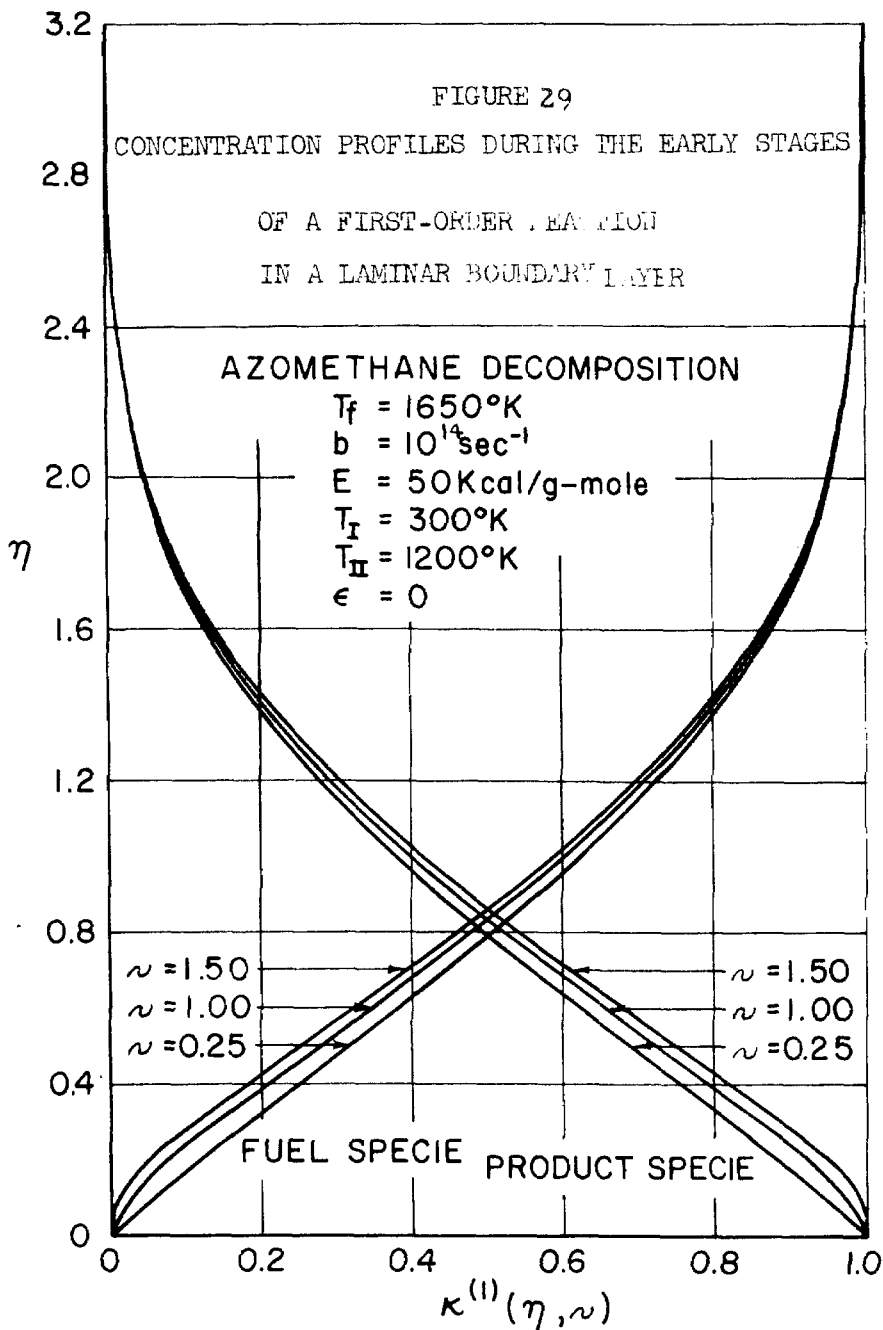
FIGURE 25

PARAMETRIC PLOT OF VARIABLES RELATED TO THE CHARACTERISTIC STAY TIME (FIRST-ORDER REACTION IN A LAMINAR BOUNDARY LAYER)









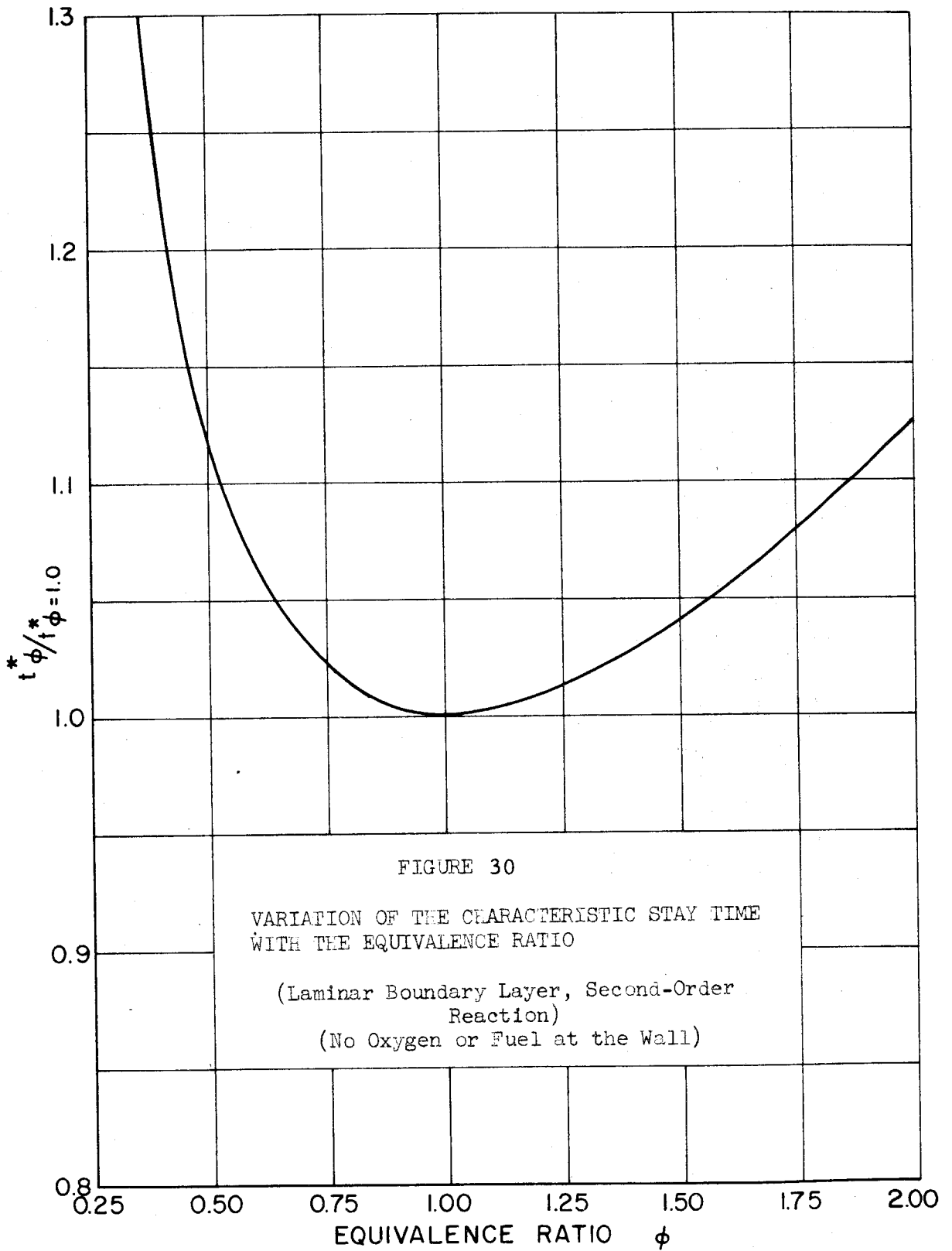


FIGURE 31

VARIATION OF THE CHARACTERISTIC STAY TIME WITH EQUIVALENCE RATIO  
(Second-order Reaction in a Laminar Boundary Layer)

NOTE: BOUNDARY CONDITIONS ASSUME EXCESS  
OXYGEN AT WALL FOR  $\phi < 1$  AND  
EXCESS FUEL AT WALL FOR  $\phi > 1$

