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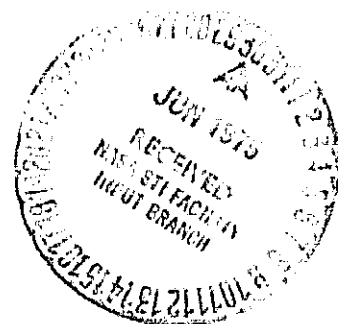   G3/34   24224

National Aeronautics and Space Administration
Office of University Affairs, Code Y
Washington, D. C.   20546

From

The Department of Physics
Southern University
Baton Rouge, Louisiana   70813

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            Principal Investigator

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The investigation of the shock structure in an ideal dissociating gas based on the formulation of continuum gas dynamics has been carried out. Please see details in the attached paper, "Shock-Wave Structure in an Ideal Dissociating Gas."

Proposed Further Investigations 1975-76

A. Investigation of "model dependency" on shock profile.

For simplicity, Lighthill's "ideal dissociating gas" model is used

for the current investigation. It will be interesting to test the

dependency of this model for the obtained results.

B. Kinetic Theory Approach

The current analysis of the shock-wave structure in an ideal dissociating

gas is based on the continuum gas dynamics. It will be interesting to

use the kinetic theory approach to investigate the same problem and then

compare their results.

Shock-Wave Structure in an Ideal Dissociating Gas*

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The shock-structure problem utilizing Lighthill's "ideal dissociating gas" model is investigated. The analysis is based on the usual formulation of continuum gas dynamics. The two extreme cases of chemical equilibrium and chemically frozen flow are investigated. Profiles for species concentration, temperature, and mean velocity are obtained for both limiting cases at various upstream conditions. The problem is also solved for arbitrary chemical reaction rates. Mathematical nature of the upstream and downstream singular points has been investigated and shock profiles for two typical chemical reaction rates are presented. As far as shock thickness is concerned, the solution for frozen flow shows good agreement with results obtained for a pure gas. Also, shock thickness based on the maximum slopes of temperature, species concentration and mean velocity, respectively, are practically the same; this is in accord with the conclusion of Talbot and Scala.

Nomenclature

a	$=$	velocity of sound
c_p	$=$	specific heat at constant pressure
c_v	$=$	specific heat at constant volume
D_{am}	$=$	binary diffusion coefficient
D_m	$=$	dissociation energy
D_t	$=$	thermal diffusion coefficient
e	$=$	specific internal energy
h	$=$	specific enthalpy
k_f	$=$	forward reaction rate constant
k_r	$=$	reverse reaction rate constant
K_m	$= \dfrac{h_m}{R_m T}$	, see equation (10)
l	$=$	mean free path
L	$=$	characteristic length
M	$=$	Mach number
p	$=$	pressure
R	$=$	Universal gas constant
T	$=$	temperature
v_i	$=$	diffusion velocity of ith species
u	$=$	mean flow velocity
W	$=$	molecular weight
X	$=$	space coordinate
Y_i	$=$	mole fraction of ith species

Greek Symbols

α_i = mass fraction of i-th. species ($\alpha_a \equiv \alpha$)

γ = adiabatic index

τ = characteristic reaction time

Δ = shock thickness

κ = compression viscosity

μ = shear viscosity

ν = frequency of the vibration mode

ρ = density

ρ_D = characteristic dissociation density

$\dot{\omega}_i$ = net rate of production of i-th species

Subscripts

$(\ )_0$ conditions at either $x = \pm\infty$

$(\ )_1$ conditions at $x = -\infty$ (upstream)

$(\ )_2$ conditions at $x = +\infty$ (downstream)

$(\ )_e$ Equilibrium Flow

$(\ )_f$ Frozen Flow

$(\ )_i$ i-th. Species

$i=a$ atomic species

$i=m$ molecular species

over a large temperature range ($10^3 \sim 7 \times 10^3$ °K), Lighthill asserts that ρ_D is practically a constant. Such a gas is termed as an "ideal dissociating diatomic gas," its rate of production for the atomic species, $\dot{\omega}$, is found to be

$$\dot{\omega} = \frac{W_m}{\Gamma} \left[(1-\alpha) \frac{\rho_D}{\rho} e^{-\frac{D_m}{R_m T}} - \alpha^2 \right] \qquad (15)$$

with

$$\Gamma = W_m^3 \left/ \left[4 k_r \rho^2 (1+\alpha) \right] \right.$$

Γ can be interpreted as a characteristic reaction time. If the chemical reaction occurs very rapidly, the value of α will differ only slightly from the local equilibrium value. In the limit of infinitely fast reaction, $\Gamma = 0$, the dynamical change of the flow field is very slow in comparison with the dissociation and recombination rates. Since the reaction rate is reversible, the flow will be isentropic[7]. At the other limit of large Γ (very slow reaction), the rate of production, $\dot{\omega}$, is effectively zero. The gas may then be considered as chemically inert and is usually referred to as chemically frozen flow. Again, the irreversibility associated with the reaction rates disappears and the flow, as in chemical equilibrium is, in fact, isentropic[7].

In any analysis of chemical non-equilibrium flow, the main difficulties arise from the coupling between the gas dynamic equations and the chemical relaxation equation. However, in the two extreme cases of frozen and equilibrium flow, the chemical relaxation equation is reduced to a very simple form, thus greatly simplifying the analysis. For the non-equalibrium case, the assumption

of Γ being a constant will be used throughout the present work. This assumption is consistent with the one made by Freeman[10].

Transport Properties

The solution of the governing equations requires a knowledge of the variation of the transport coefficients; shear viscosity μ, thermal conductivity λ, binary diffusion coefficient D_{am}, and co-efficient of thermal diffusion D_t, with temperature and concentration. For an actual engineering problem, experimental data may be used; but, for the case of an idea dissociating gas mixture of dia-tomic molecules, a simplified kinetic theory approximation can be made.

Following Dorrance[11], we approximate the viscosity and thermal conductivity by

$$\mu = \sum_i \mu_i y_i \quad , \quad \lambda = \sum_i \lambda_i y_i$$

with y_i, the mole fraction of each species. For a binary mixture of atoms and molecules, μ and λ are

$$\mu = \mu_m \frac{1-\alpha}{1+\alpha} + \mu_a \frac{2\alpha}{1+\alpha}$$

$$\lambda = \lambda_m \frac{1-\alpha}{1+\alpha} + \lambda_a \frac{2\alpha}{1+\alpha}$$

respectively. Accurate to the first order approximation in solving the Boltzmann equation through the Chapman-Enskog procedure, we may further prescribe that

$$\mu_m \simeq \mu_a,$$

thus,

$$\mu \simeq \mu_m \simeq \mu_a .$$

A first order approximation to the thermal conductivity for a monotomic gas is given by Penner[12]

$$\lambda_a = \frac{15}{4} R_a \mu_a$$

For a pure polytropic gas, the thermal conductivity may be approximated[12] by

$$\lambda_m = \frac{15}{4} R_m \mu_m \left(\frac{1}{3} + \frac{4}{15} \frac{C_{p,m}}{R_m} \right)$$

The factor in parenthesis is known as the Eucken approximation which accounts for the transfer of energy between the translational and rotational degrees of freedom when polytropic molecules collide. Approximating the specific heats at constant pressure, namely $C_{p,m}$ and $C_{p,a}$, by their values for chemically frozen flow, one finds

from the caloric equation of state that

$$C_{p,f} = \alpha C_{p,a} + \alpha_m C_{p,m} = \left[K_m + (5 - K_m)\alpha \right] R_m \tag{16}$$

hence

$$\lambda = \frac{\mu R_m}{4(1+\alpha)} \cdot \left[(5 + 4 K_m) + (55 - 4 K_m)\alpha \right]$$

$$= \lambda_a \cdot \frac{(5 + 4 K_m) + (55 - 4 K_m)\alpha}{30 (1+\alpha)} \tag{17}$$

Eq.(17) implies that, although the mixture viscosity μ may be assumed the same as that for the atomic species, the thermal conductivity λ will be less than λ_a by a factor of about 2/3, since K_m varies between 7/2 and 9/2.

The Prandtl number Pr, through combining Eq.(16) and (17), becomes

$$Pr = \frac{\mu C_{pf}}{\lambda} = \frac{4(1+\alpha)\left[K_m + (5-K_m)\alpha\right]}{(5+4K_m) + (55-4K_m)\alpha} \tag{18}$$

Taking the average value of K_m, $K_m \simeq 4$, one finds that for α varying from zero to one, Pr from Eq.(18) varies from 16/21 to 40/60.

Using the thermal equation of state to express density in terms of other thermodynamic variables, we have the Schmidt number Sc.

$$Sc = \frac{\mu}{\rho D_{am}} = \frac{\mu_m}{\rho D_{am}} (1+\alpha) R_m T$$

Assuming that ρD_{am} is independent of composition, it may be evaluated at $\alpha = 0$, Hence, we obtain

$$Sc = \left(\frac{\mu_m}{\rho_m D_{am}}\right)_{\alpha=0} \cdot (1+\alpha) \simeq (1+\alpha) \tag{19}$$

The thermal diffusion coefficient D_t may be expressed in terms of the binary diffusion coefficient D_{am} [12].

$$D_t = k_t D_{am} \tag{20}$$

Theoretical results for k_t based on kinetic theory are very complex but to an acceptable approximation[12]

$$k_t = 0.35 \frac{W_m - W_a}{W_m + W_a} y_a y_m$$

In the case of a pure diatomic gas

$$k_t = 0.234 \frac{\alpha(1-\alpha)}{(1+\alpha)^2}$$

thus from Eq.(20),

$$D_t = 0.234 \frac{\alpha(1-\alpha)}{(1+\alpha)^2} D_{am}$$

The coefficient $D_t/\rho D_{am}$ appearing in the diffusion velocity [see Eq.(24)] may be written as -

$$\frac{D_t}{\rho D_{am}} = \frac{W_a W_m}{\overline{W}^2} k_t$$

Since

$$\frac{W_a W_m}{\overline{W}^2} = \frac{(1+\alpha)^2}{2}$$

therefore

$$\frac{D_t}{\rho D_{am}} = 0.117 \, \alpha \, (1-\alpha).$$

Governing Equation in Dimensionless Form

Governing equations are normalized by introducing the following set of dimensionless quantities:

$$v = mu/P \qquad \text{(velocity)}$$
$$\tau = m^2 R_m T/P^2 \qquad \text{(temperature)}$$
$$A = mQ/P^2 \qquad \text{(shock strength)}$$
$$\tau_D = m^2 D_m/P^2 \qquad \text{(dissociation energy)}$$
$$\overline{\Gamma} = mT/L W_m \qquad \text{(chemical reaction time)}$$
$$X = \frac{4}{3} + \frac{\kappa}{\mu} \qquad \text{(viscosity)}$$

and the characteristic length, $L \equiv \mu/m$.

Thus, the continuity equation for the atomic species, the momentum equation, and the energy equation become

$$L \frac{d}{dx}\left(\alpha + \frac{\rho_a u_a}{m}\right) = \frac{1}{\overline{\Gamma}}\left[(1-\alpha)\frac{\rho_D}{\rho} e^{-\frac{\tau_D}{\tau}} - \alpha^2\right] \tag{21}$$

$$XL \frac{dv}{dx} = V + (1+\alpha)\frac{\tau}{v} - 1 \tag{22}$$

$$[(K_m-1) + (4-K_m)\alpha]\tau + \alpha\tau_D - \frac{v^2}{2} + v - \frac{[K_m + (5-K_m)\alpha]}{\rho_a}\frac{d\tau}{dx}$$

$$+ \left[(5-K_m)\tau + \tau_D\right]\frac{\rho_a u_a}{m} = \frac{A}{2} \tag{23}$$

respectively. In Eq.(23) the term due to the diffusion velocity $\rho_a u_a / m$ is given by

$$\frac{\rho_a u_a}{m} = -\left(\frac{1}{Sc}\right) \left\{ \left[1 + \frac{\alpha(1-\alpha)}{2}\right]\frac{d\alpha}{dx} + \left[\frac{D_t}{\rho D_{am}} + \frac{\alpha(1-\alpha^2)}{2}\right]\frac{L}{\tau}\frac{d\tau}{dx} + \right.$$
$$\left. - \frac{\alpha(1-\alpha^2)}{2}\frac{L}{V}\frac{dV}{dx} \right\} \tag{24}$$

This set of equations for V, τ and α ; the boundary conditions prescribed at upstream and downstream of the shock wave

$$\frac{dV}{dx} = \frac{d\tau}{dx} = \frac{d\alpha}{dx} = 0 \qquad at \quad x = \pm\infty$$

and the transport properties of the gas: λ, μ, D_t, D_{am}, X completely define the shock structure problem.

The set of governing equations for the three cases that we shall investigate can now be listed as follows:

(A) Equilibrium flow $(\bar{\Gamma} = 0)$

Species Continuity Equation:

Since $\bar{\Gamma} = 0$ in Eq.(21) the term in brackets must also be zero, thus the equilibrium mass fraction is given by

$$\frac{\alpha^2}{1-\alpha} = \frac{\rho_D}{\rho} e^{-\frac{\tau_D}{\tau}} \tag{25}$$

which is merely the repetition of Eq.(14).

Momentum Equation:

$$XL\frac{dV}{dx} = V + (1+\alpha)\frac{\tau}{V} - 1 \tag{26}$$

Energy Equation:

Substitution of Eqs.(24)(25) into (23) gives

$$\left\{ \frac{1}{Pr}\left[K_m + (5-K_m)\alpha\right] + \frac{1}{Sc}\left(5 - K_m + \frac{\tau_D}{\tau}\right)\left[\frac{\alpha(1-\alpha^2)}{2}\left(1 + \frac{\tau_D}{\tau}\right) + \frac{D_t}{\rho D_{am}}\right] \right\}\frac{L}{\tau}\frac{d\tau}{dx}$$
$$= \left[(K_m - 1) + (4 - K_m)\alpha\right]\tau + \alpha\tau_D - \frac{V^2}{2} + V - \frac{A}{2} \tag{27}$$

(B) Frozen Flow ($\bar{\Gamma} \to \infty$)

Species Continuity Equation:

$$L\left[1 + \frac{\alpha(1-\alpha)}{2}\right]\frac{d\alpha}{dx} = \frac{1}{L}(\alpha - \alpha_1) + \frac{\alpha(1-\alpha^2)}{2} \cdot \frac{L}{V} \cdot \frac{dv}{dx} +$$

$$- \left[\frac{D_t}{\rho D_{am}} + \frac{\alpha(1-\alpha^2)}{2}\right]\frac{L}{\tau} \cdot \frac{d\tau}{dx} \qquad (28)$$

Momentum Equation:

$$XL\frac{dv}{dx} = v + (1+\alpha)\frac{\tau}{v} - 1 \qquad (29)$$

Energy Equation:

$$\frac{1}{Pr}\left[K_m + (5-K_m)\alpha\right]L\frac{d\tau}{dx} = \left[(K_m-1) + (5-K_m)\alpha_1 - \alpha\right]\tau + v +$$

$$- \frac{v^2}{2} + \alpha_1 \tau_D - \frac{A}{2} \qquad (30)$$

(C) Non-Equilibrium Flow

The terms related to the diffusion velocity in the species continuity equation and the energy equation will be neglected in the case of finite chemical reaction time. The simplification due to this assumption is obvious, since the species continuity equation is hence reduced to a first order differential equation. The assumption is justified from the results for the frozen flow case where the change in concentration, caused only by diffusion, is found to be very small. In addition, the chemical reaction time $\bar{\Gamma}$ is taken to be constant throughout the shock wave. Then, the set of governing equations becomes

$$L\frac{d\alpha}{dx} = \frac{1}{\bar{\Gamma}}\left[(1-\alpha)\frac{\rho_D}{\rho} e^{-\frac{\tau_D}{\tau}} - \alpha^2\right] \qquad (31)$$

$$XL\frac{dv}{dx} = v + (1+\alpha)\frac{\tau}{v} - 1 \qquad (32)$$

$$\frac{1}{P_r} \left[K_m + (5-K_m)\alpha \right] L \cdot \frac{d\tau}{dx} = \left[(K_m-1) + (4-K_m)\alpha \right] \tau + \alpha \tau_D - \frac{V^2}{2} + V - \frac{A}{2} \qquad (33)$$

Mach Number

The basic parameter in the shock Structure Problem is always the upstream Mach number, $M = u/a$, in which the speed of sound a is

$$\sqrt{\Upsilon (1+\alpha) R_m T}$$

Since the adiabatic index, Υ, is not defined in a simple way if concentration changes are allowed.

For the case of frozen flow

$$\Upsilon_f = \frac{K_m + (5-K_m)\alpha}{(K_m-1) + (4-K_m)\alpha}$$

In the case of equilibrium flow, Clarke[13] gives the ratio Υ_e/Υ_f for $K_m = 4$ to be

$$\frac{\Upsilon_e}{\Upsilon_f} = \left(\frac{a_e}{a_f}\right)^2 = \left\{ 1 + \frac{\alpha(1-\alpha)}{3} \cdot \frac{[(\tau_D+1)(1+\alpha) - (4+\alpha)]^2}{(\tau_D+1)^2 \alpha (1-\alpha^2) + 2(4+\alpha)} \right\}^{-1}$$

One can see then

$$\Upsilon_e \leq \Upsilon_f$$

Since the frozen and equilibrium situations represent the two extremes of chemical behavior, the adiabatic index for the non-equilibrium flow will be bounded between Υ_f and Υ_e. We have, therefore, three different speeds of sound making the standard definition of the Mach number somewhat ambiguous. To circumvent the complications that could arise from this ambiguity, we adopt the flow parameter ΥM^2 which is applicable to all three flow situations.

$$\Upsilon M^2 = \frac{u^2}{(1+\alpha) R_m T} = \frac{V}{(1+\alpha)\tau}$$

At upstream as $x \longrightarrow -\infty$.

$$(\Upsilon M^2)_1 = \frac{V_1}{(1+\alpha_1)\tau_1}$$

Substitution of the momentum equation gives

$$(\Upsilon M^2)_1 = \frac{V_1}{1-V_1} \qquad \text{or} \qquad V_1 = \frac{(\Upsilon M^2)_1}{1+(\Upsilon M^2)_1}$$

Therefore, in the present analysis $(\Upsilon M^2)_1$, or V_1 will be used as the basic parameter. Herein, this parameter is assumed to lie in a range where the existence of a compressive shock wave is assured. In other words, the strength of the shock wave is large enough to give a continuous shock profile for the all values of $\bar{\Gamma}$.

Rankine-Hugoniot Relations

Since the gradients of all physical quantities vanish at a large distance upstream and downstream of the shock wave, conditions at end points for equilibrium and non-equilibrium flows are the same. The end consitions for frozen flow are different due to the fact that the concentration downstream of the shock wave remains the same as the upstream value.

(A) Equilibrium Flow

Setting all gradients zero in Eqs.(26,27), we find the normalized velocity at end points to be

$$V_{1,2} = \frac{\beta_e}{1+\beta_e} \left[1 \pm \frac{\beta_e - 1}{2\beta_e} E_e \right] \tag{34}$$

where

$$\beta_e = -\frac{K_m + (5-K_m)\alpha}{(K_m-1) + (4-K_m)\alpha}$$

$$E_e = \frac{2\beta_e}{\beta_e - 1} \left[1 - \frac{2(\beta_e^2 - 1)}{\beta_e^2} \left(\frac{\dot{h}}{2} - \alpha_1 \tau_2 \right) \right]^{-\frac{1}{2}}$$

The plus sign in Eq.(34) is associated with the upstream point, $x = +\infty$, while the minus sign should be taken for the downstream point, $x = -\infty$. Through the momentum equation, Eq.(26), we find the normalized temperature at end points to be

$$\tau_{1,2} = \frac{V_{1,2}\left(1 - V_{1,2}\right)}{1 + \alpha_{1,2}} \tag{35}.$$

The concentration $\alpha_{1,2}$ is then found by knowing τ_1 and τ_2 through the species continuity equation, Eq.(25). Eqs.(25,34,35) are solved simultaneously to determine v, τ, and α at the two state points. For illustration, Figs.1,2,3 present the results for shock waves of various strength characterized by $(\gamma M^2)_1$. It is interesting to note that both the velocity ratio and the temperature ratio for a given upstream Mach number do not vary monotonically with respect to the change of upstream atomic concentration.

(B) Frozen Flow

The conditions for the frozen flow case differ in that the mass fraction α is the same at $x = \pm\infty$. Since the upstream conditions represent an equilibrium state, the downstream state conditions (α_2, V_2, τ_2) do not in general represent an equilibrium state. Thus, the flow after passing through the shock must make a transition to an equilibrium state behind the shock. This relaxation zone, analogous to shock transition in a two-phase (solid-gas) fluid, will not be discussed in the present analysis. Readers are referred to a text book on physical gasdynamics for further discussions.[14]

Hence, instead of having Eq.(25) for the concentration, we now have the condition

$$\alpha_1 = \alpha_2 = \alpha_0$$

together with the momentum equation and the energy equation. Setting all gradients to zero, we obtain the normalized velocity at both end points

$$V_{1,2} = \frac{\beta_f}{1 + \beta_f} \left[1 \pm \frac{\beta_f - 1}{2\beta_f} E_f \right] \tag{36}$$

where

$$\beta_f = \frac{K_m + (5 - K_m)\alpha_o}{(K_m - 1) + (4 - K_m)\alpha_o}$$

$$E_f = \frac{2\beta_f}{\beta_f - 1} \left[1 - \frac{2(\beta_f^2 - 1)}{\beta_f^2}\left(\frac{A}{2} - \alpha_o \tau_p \right) \right]^{\frac{1}{2}}$$

Again, the plus sign should be adopted for $x = -\infty$; the minus sign for $x = +\infty$. The normalized temperature at two end points is

$$\tau_{1,2} = \frac{V_{1,2}(1 - V_{1,2})}{1 + \alpha_o} .$$

A comparison of Eq.(34) and Eq.(36) shows the only difference in $V_{1,2}$ between equilibrium and frozen flow is the replacement of β_c in the former case by β_f in the latter case. Since the concentration α is unchanged for frozen flow, β_f is thus constant, the values of all physical variables at end points for frozen flow can therefore be obtained without numerical iteration. The parameter, E_f, which is also constant may be written as

$$E_f = \frac{2\beta_f}{\beta_f - 1} \left[\frac{M_{f1}^2 - 1}{1 + \gamma M_{f1}^2} \right]$$

in which M_{f1} is the upstream frozen flow Mach number.

Here

$$E_f = 0 \quad \text{for} \quad M_{f1} = 1,$$

and

$$E_f = \frac{2}{\beta_f - 1} \quad \text{for} \quad M_{f1} \to \infty,$$

thus

$$0 \leqslant E_f \leqslant \frac{2}{\beta_f - 1} .$$

Phase-Space Analysis.

It is a characteristic feature of the shock structure problem that state points at upstream and downstream are unavoidably singular points with regard to the set of governing equations. Phase-space analysis is the usual technique applied to assure the uniqueness of the solution mathematically, and in practice to obtain an initial slope to start the numerical integration. Analysis in the two dimensional phase plane has been a standard procedure, while the investigation in three or more dimensional phase space is by no means a simple routine. The classical treatise of Poincaré[15] defined the nature of singularities in three dimensions, but did not illustrate the procedure with practical problems. The present analysis follows the path set forth by Talbot and Sherman[2] in their investigation of the shock structure problem based on continuum gasdynamics, taking into account the higher-order Burnett stresses.

For an autonomous system of three non-linear ordinary differential equation governing v, τ, and α, we have

$$\left. \begin{aligned} A \, \frac{d\alpha}{d\chi} &= F(\alpha, v, \tau) \\ B \, \frac{dv}{d\chi} &= G(\alpha, v, \tau) \\ C \, \frac{d\tau}{d\chi} &= H(\alpha, v, \tau) \end{aligned} \right\} \quad (37)$$

where A, B, C are simply constants, which, if one prefers, may be absolved in F, G, and H, respectively. The boundary conditions at end points are such that

$$F(\alpha_0, v_0, \tau_0) = G(\alpha_0, v_0, \tau_0) = H(\alpha_0, v_0, \tau_0) = 0,$$

thus making the slopes $d\alpha/dv$, $d\tau/dv$ indeterminate at end points.

Introduce

$$\tilde{\alpha} = \alpha - \alpha_0 = \tilde{\alpha}_0 e^{b\sigma}$$

$$\tilde{v} = v - v_0 = \tilde{v}_0 e^{b\sigma}$$

$$\tilde{\tau} = \tau - \tau_0 = \tilde{\tau}_0 e^{b\sigma}$$

$$\tag{38}$$

with $\tilde{\alpha}_0, \tilde{v}_0, \tilde{\tau}_0$ being constants, σ a parameter along the integral curve, b a characteristic root. In the neighborhood of the singular points, Eqs.(37) and (38) give us a system of algebraic equations governing $\tilde{\alpha}_0, \tilde{v}_1, \tilde{\tau}_0$.

$$
\begin{bmatrix}
-Ab + F_\alpha & F_v & F_\tau \\
G_\alpha & -Bb + G_v & G_\tau \\
H_\alpha & H_v & -Cb + H_\tau
\end{bmatrix}
\begin{bmatrix}
\tilde{\alpha}_0 \\
\tilde{v}_0 \\
\tilde{\tau}_0
\end{bmatrix}
= [0]
\tag{39}
$$

where $F_\alpha \equiv \left(\dfrac{\partial F}{\partial \alpha}\right)_0$, $F_v \equiv \left(\dfrac{\partial F}{\partial v}\right)_0$, etc. To have a set of non-trivial $\tilde{\alpha}_0, \tilde{v}_0$ and $\tilde{\tau}_0$, the determinant of the square matrix in Eq.(39) must vanish, thus resulting in a cubic equation for b.

$$(ABC)b^3 - [ACG_v + ABH_\tau + BCF_\alpha]b^2 +$$

$$+ [A(G_v H_\tau - G_\tau H_v) + B(F_\alpha H_\tau - F_\tau H_\alpha) + C(F_\alpha G_v - F_v G_\alpha)]b + \tag{40}$$

$$+ [F_v(G_\alpha H_\tau - G_\tau H_\alpha) + F_\alpha(G_\tau H_v - G_v H_\tau) + F_\tau(G_v H_\alpha - G_\alpha H_v)] = 0$$

In general, three different roots of b are obtained, among which one value of b should be selected; according to which a set of $\tilde{\alpha}_0, \tilde{v}_1, \tilde{\tau}_0$ is computed. The selection of this particular b is illustrated in the following calculation.

(A) Equilibrium flow

Since in this limiting case the mass fraction may be written in terms of the velocity and temperature, the number of independent variables is reduced to two. Thus, in the set of equations [Eq.(37)] we have, equivalently,

$$F(\alpha, v, \tau) = 0.$$

Or $\qquad\qquad \dfrac{C}{B} \cdot \dfrac{d\tau}{dv} = \dfrac{H}{G}$ $\qquad\qquad\qquad\qquad$ (41)

One can also show that the cubic equation, Eq.(40), is reduced to a quadratic. An analysis of the two roots, b_1, b_2, of this quadratic at each of the state points reveals that the downstream point, $x=+\infty$, is invariably a saddle point; and the upstream singular point, $x=-\infty$, is an unstable node. In other words, the ratio b_1/b_2 at $x=+\infty$ is negative, thus signifying a saddle point; it is positive at $x=-\infty$, thus signifying a nodel point.

Take a typical example where the upstream atomic concentration α_1 is 0.183; we sketch the variation of b as a function of the normalized upstream or downstream velocity in Fig.4. There is a downstream velocity v_2 associated with every given upstream velocity v_1. One root remains positive for all values of v_1 and v_2, the second root passes through zero at a certain value of v where $v_1=v_2$, or the upstream Mach number based on equilibrium sound speed is approximately unity. The second root is obviously the characteristic root of interest, since there should be no shock wave of finite strength at equilibrium Mach number of unity. One also observes from Fig.4 that the value of b reaches a maximum and a minimum when $v_1 > 0.9$. This behavior need not concern us, as the corresponding Mach number for $v_1 > 0.9$ is so high that the model of ideal dissociating gas breaks down long before the situation arises.

Having determined the state conditions at end points and the initial slope, Eq.(41) can be integrated numerically in a routine manner.

(B) Frozen Flow

Unlike the preceding example where the algebraic equation (Eq.(40)) for b is reduced to a quadr tic, the present case has a cubic equation governing b. The b versus V_1 variation is presented in Fig.5 for two different upstream conditions: $\alpha_1 = 1$ and $\alpha_t = 0$. Three real roots of b are obtained, among them one is chosen based on the same reasoning as given in the preceding section. The selected value of b used in numerical integration cuts across the b=0 line at two different places for $\alpha_1 = 1$ and $\alpha_1 = 0$; because the definition of upstream Mach number depends on the upstream atomic concentration. Once a proper value of b is selected, the integration proceeds from the downstream point toward the upstream and point.

(C) Non-Equilibrium Flow

Eq.(40) is again solved for two examples where the reaction time $\bar{T}$ is 5 and 2 respectively. Results are presented in Fig.6. Three real roots of b are obtained, the selected value of b for integration is the one which crosses b=0 at $M_{f1} \approx 1$. The integration starts from downstream end point and proceeds toward the upstream end point.

Numerical Results

(A) Shock Profiles

Shock profiles for an example of $(\gamma M^2)_1 = 10$ and $\alpha_1 = 0.183$ are presented in Fig.7, in which a very pronounced overshoot in concentration ratio is recorded, while the temperature profile varies only monotonically. As the reaction time $\bar{T}$ increases from zero (equilibrium flow) to a value of 2 and then 5, we find in Fig.8 and 9 a temperature overshoot which increases with $\bar{T}$. In the limiting case of frozen flow, $\bar{T} \rightarrow \infty$, the shock profile again records a

monotonic variation for the temperature, but a high peak for the profiles of the concentration ratio. In this case, the concentration ratio changes purely due to mass diffusion, not because of chemical reaction as in the case of $\bar{\Gamma} = 0$.

(B) Shock Wave Thickness

The most commonly employed definition of the shock thickness is

$$\Delta = \frac{(\Delta v)_{1,2}}{\left|\frac{dv}{dx}\right|_{max.}} \tag{42}$$

where $\left|\frac{dv}{dx}\right|$ max is the maximum slope of the velocity profile and $(\Delta v)_{1,2}$ is the total change in v. For comparison with previous investigators, it is convenient to obtain shock thicknesses in terms of mean free path evaluated at the upstream state point. The mean free path for Maxwell molecules is

$$l_1 = \frac{16}{5} \cdot \frac{\mu_1}{\rho_1 \sqrt{2\pi R T_1}}$$

Assuming the temperature dependence of viscosity is given by*

$$\mu = \mu_1 \left(\frac{T}{T_1}\right)^S = \mu_1 \left(\frac{\tau}{\tau_1}\right)^S$$

the ratio L/l_1 is determined to be

$$\frac{L}{l_1} = \frac{\sqrt{50\pi}}{16} \cdot \frac{(\tau/\tau_1)^S}{(\gamma M^2)_1^{1/2}}$$

where the characteristic length, L, as defined previously is $L = \frac{\mu}{\rho_1 u_1}$.

---

* Though S should be unity in consistency with the assumption of Maxwell molecules, it is not uncommon to assign S some other value to account for the departure of real gas from the Maxwell model.

The expression for the shock thickness in units of mean free path becomes

$$\frac{\Delta}{l_1} = \frac{(\Delta V)_{1,2}}{\frac{16}{\sqrt{50\pi}} \cdot \frac{(\gamma M^2)_1^{1/2}}{(\tau/\tau_1)^S} \cdot \left| \frac{dv}{d(x/L)} \right|_{max}} \qquad (43)$$

in the present analysis the exponent S was taken to have the value 0.5.

Figure 11 shows the variation of the ratio l_1/Δ with $(\gamma M^2)_1$ for both chemically frozen and equilibrium flow. It is apparent that the value of l_1/Δ for the equilibrium case is greater than that for the frozen flow condition at a specific value of $(\gamma M^2)_1$. In other words, for a given upstream condition the shock thickness based on maximum slope is greater for the frozen flow case than for the equilibrium situation. For the equilibrium case, the thickness, Δ, for a given value of $(\gamma M^2)_1$ first decreases then increases as the atomic concentration is increased. A similar type of behavior was previously noted in the determination of the upstream and downstream conditions in equilibrium flow. This suggests that for a given value of $(\gamma M^2)_1$ the thickness, Δ, has a maximum as the atomic mass fraction is increased from zero to unity. Fig.12 shows that this is indeed the case for flow in chemical equilibrium.

Fig.13 gives a comparison of the results from the present study with previous investigators. As expected, the solution for frozen flow shows good agreement with results obtained for a pure gas.

Talbot and Scala[6] define a shock thickness based on any flow property, f.

$$\Delta_f = \frac{f_{max.} - f_{min.}}{\left| \frac{df}{d\left(\frac{X}{L}\right)} \right|_{max.}}$$

Fig.14 shows the variation with $(\gamma M')_1$ of the maximum slope thickness based on v, τ, and α for both frozen and equilibrium flow. It should be noted that the definition of Δ_f in Fig.14 is slightly different from the preceding equation, as the factor $f_{max} - f_{min.}$ is replaced by $\left| f_1 - f_2 \right|$; yet the quantitative discrepancy in Δ_f based on any physical quantity, even if it has an overshoot in the shock layer, is always negligible. It can be seen that different properties predict shock thicknesses of the same order of magnitude; this is in agreement with the conclusions of Talbot and Scala.

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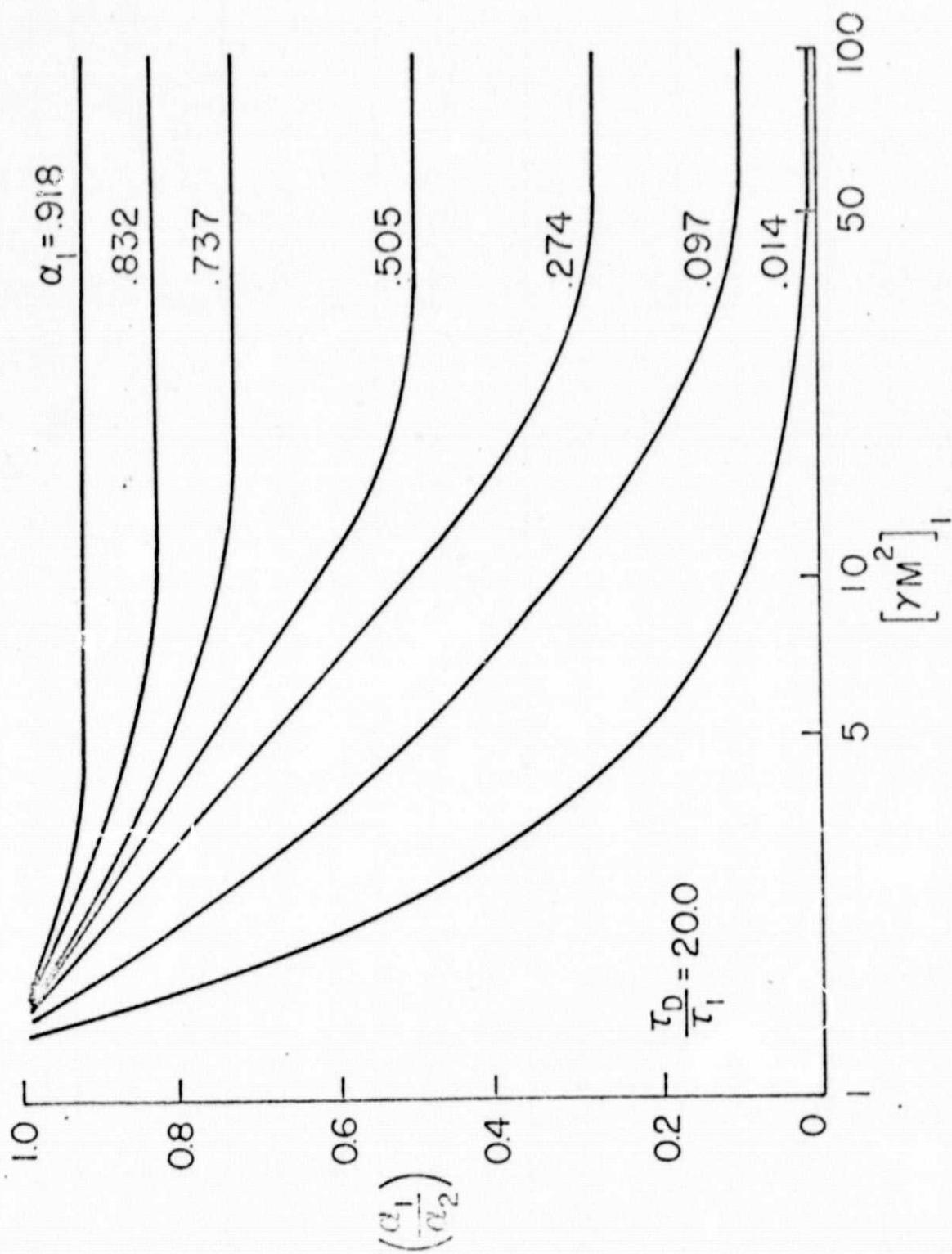
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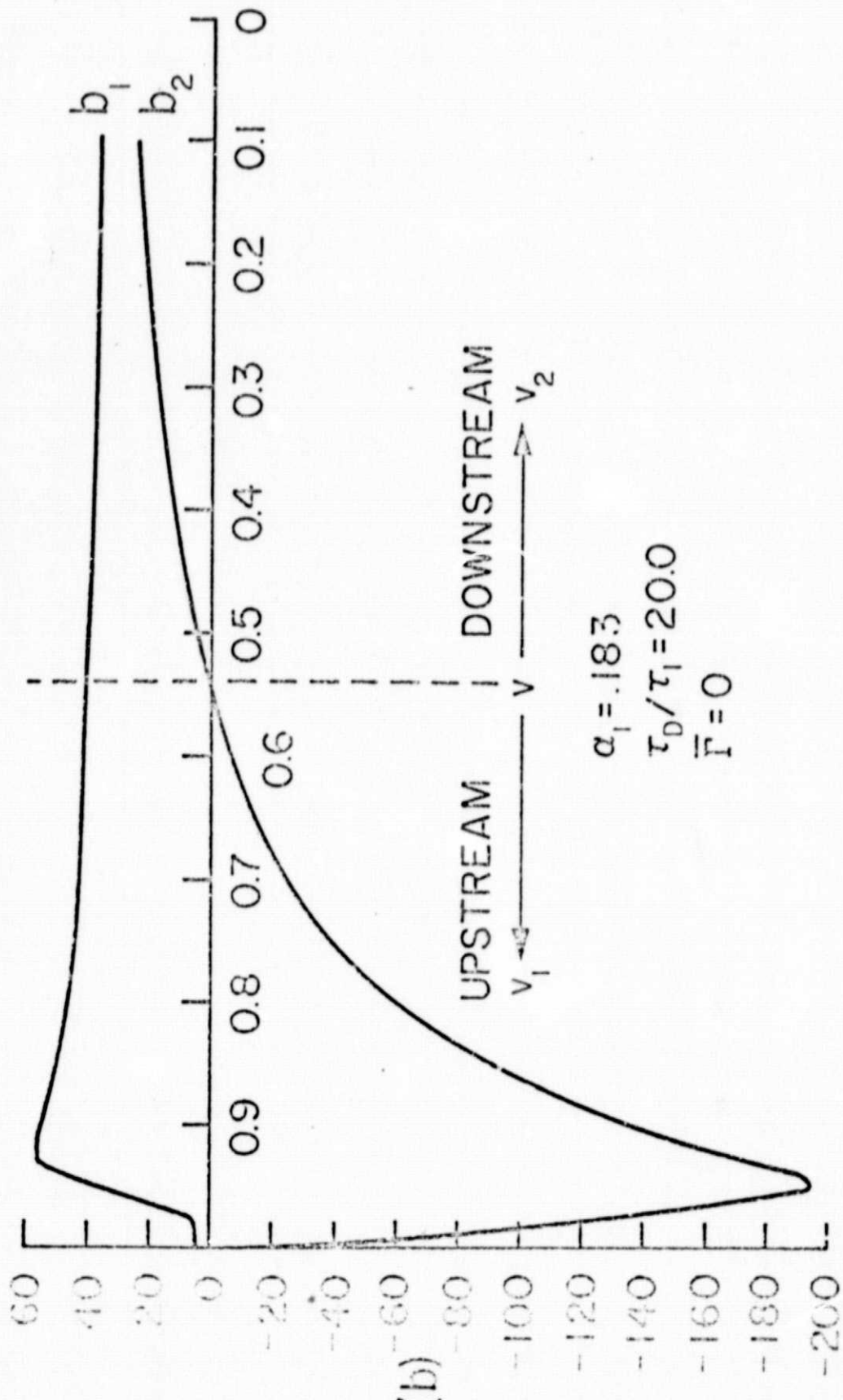
FIGURE CAPTIONS

Fig 1.   VELOCITY RATIO $\frac{V_1}{V_2}$ FOR EQUILIBRIUM FLOW

Fig 2.   TEMPERATURE RATIO $\frac{T_1}{T_2}$ FOR EQUILIBRIUM FLOW

Fig 3.   CONCENTRATION RATIO $\frac{\alpha_1}{\alpha_2}$ FOR EQUILIBRIUM FLOW

Fig 4.   CHARACTERISTIC ROOTS (b_1, b_2) FOR EQUILIBRIUM FLOW

Fig 5.   CHARACTERISTIC ROOTS (b_1, b_2, b_3) FOR FROZEN FLOW

Fig 6.   CHARACTERISTIC ROOTS (b_1, b_2, b_3) FOR NON-EQUILIBRIUM FLOW

Fig 7.   SHOCK PROFILES FOR EQUILIBRIUM FLOW

Fig 8.   SHOCK WAVE PROFILES FOR NON-EQUILIBRIUM FLOW

Fig 9.   SHOCK WAVE PROFILES FOR NON-EQUILIBRIUM FLOW

Fig 10. SHOCK WAVE PROFILES FOR FROZEN FLOW

Fig 11. SHOCK THICKNESS FOR EQUILIBRIUM AND FROZEN FLOW

Fig 12. SHOCK THICKNESS FOR EQUILIBRIUM FLOW

Fig 13. COMPARISON OF SHOCK THICKNESS WITH PREVIOUS INVESTIGATORS
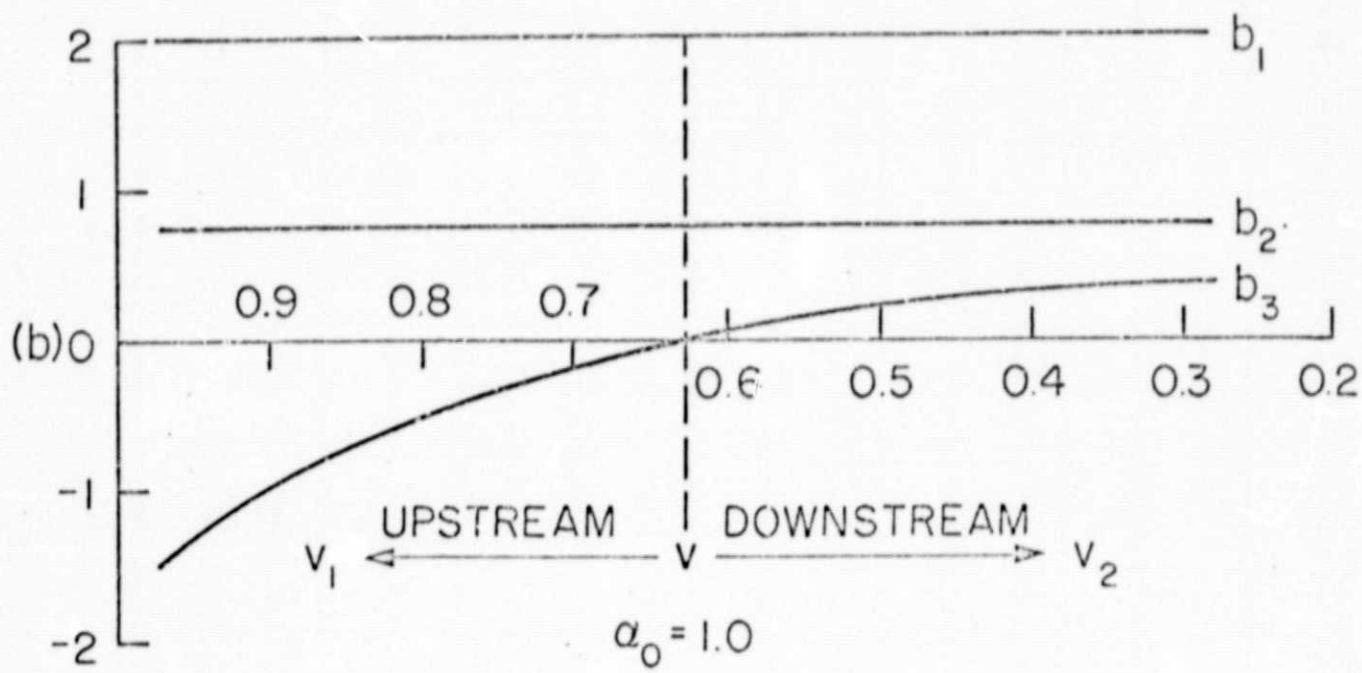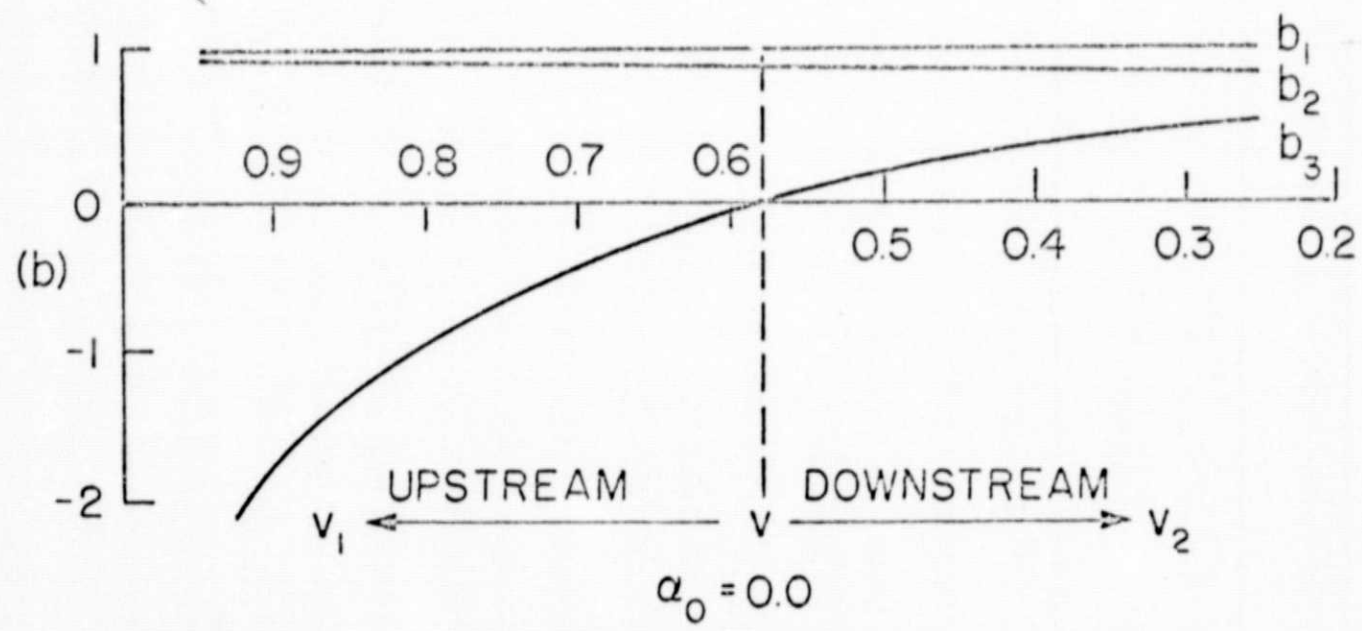
Fig 14. MAXIMUM SLOPE THICKNESS BASED ON α, T AND V.

(b)

$\alpha_0 = 1.0$

$\alpha_0 = 0.0$

(l)

$\left[\gamma M^2\right]_1 = 10.0$

$\alpha_1 = .183$

$\tau_D/\tau_1 = 20.0$

$\overline{\Gamma} = 0$

$[\gamma M^2]_1 = 10.0$

$\alpha_1 = .183$

$\tau_D/\tau_1 = 20.0$

$\overline{\Gamma} = 2.0$

$[\gamma M^2]_1 = 10.0$

$\alpha_1 = .183$

$\tau_D / \tau_1 = 20.0$

$\bar{\Gamma} = 5.0$

τ / τ_2

α / α_2

V / V_1

(X/L)

$[\gamma M^2]_1 = 10.0$

$\alpha_1 = \alpha_2 = \alpha_0 = .183$

$\overline{\Gamma} = \infty$
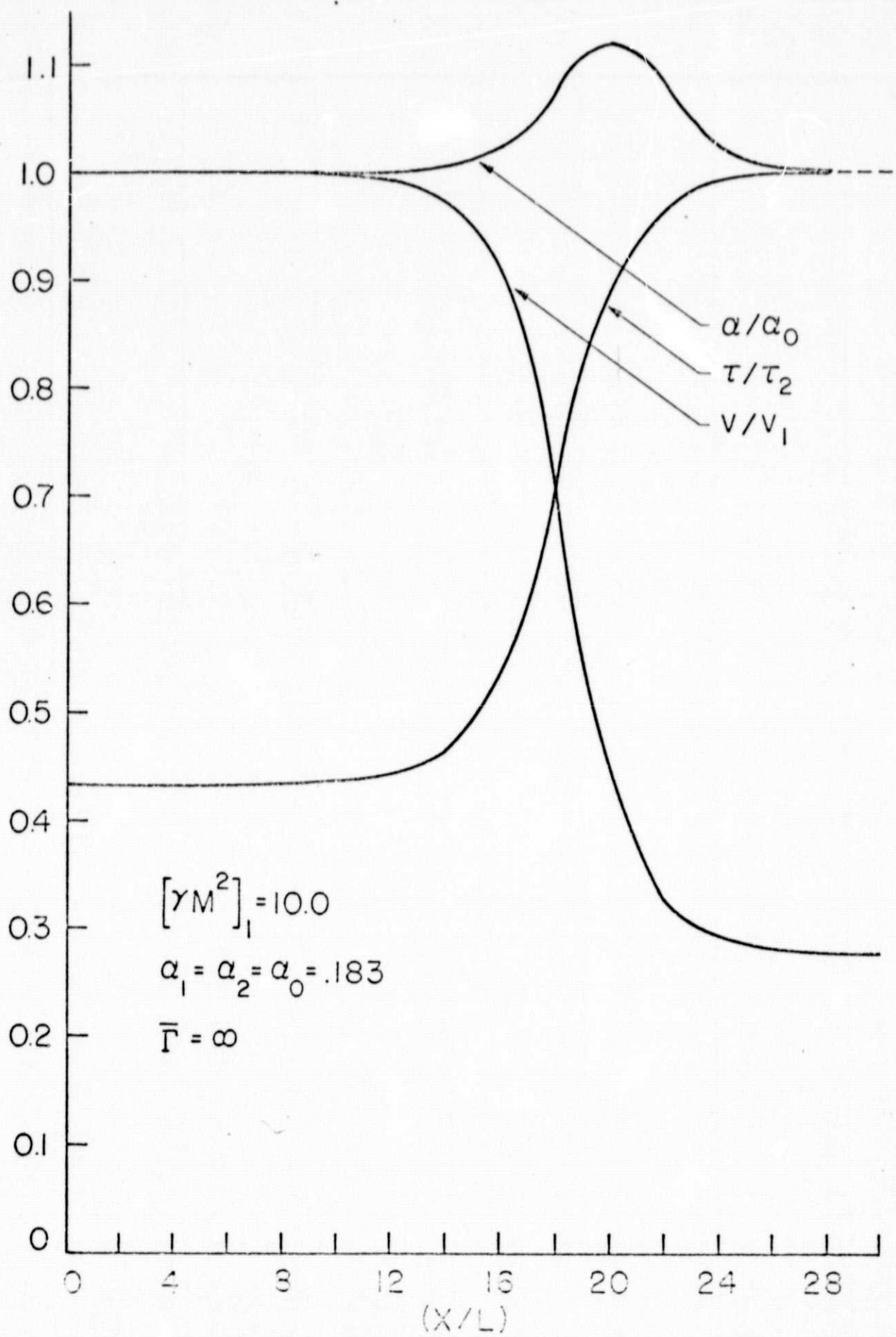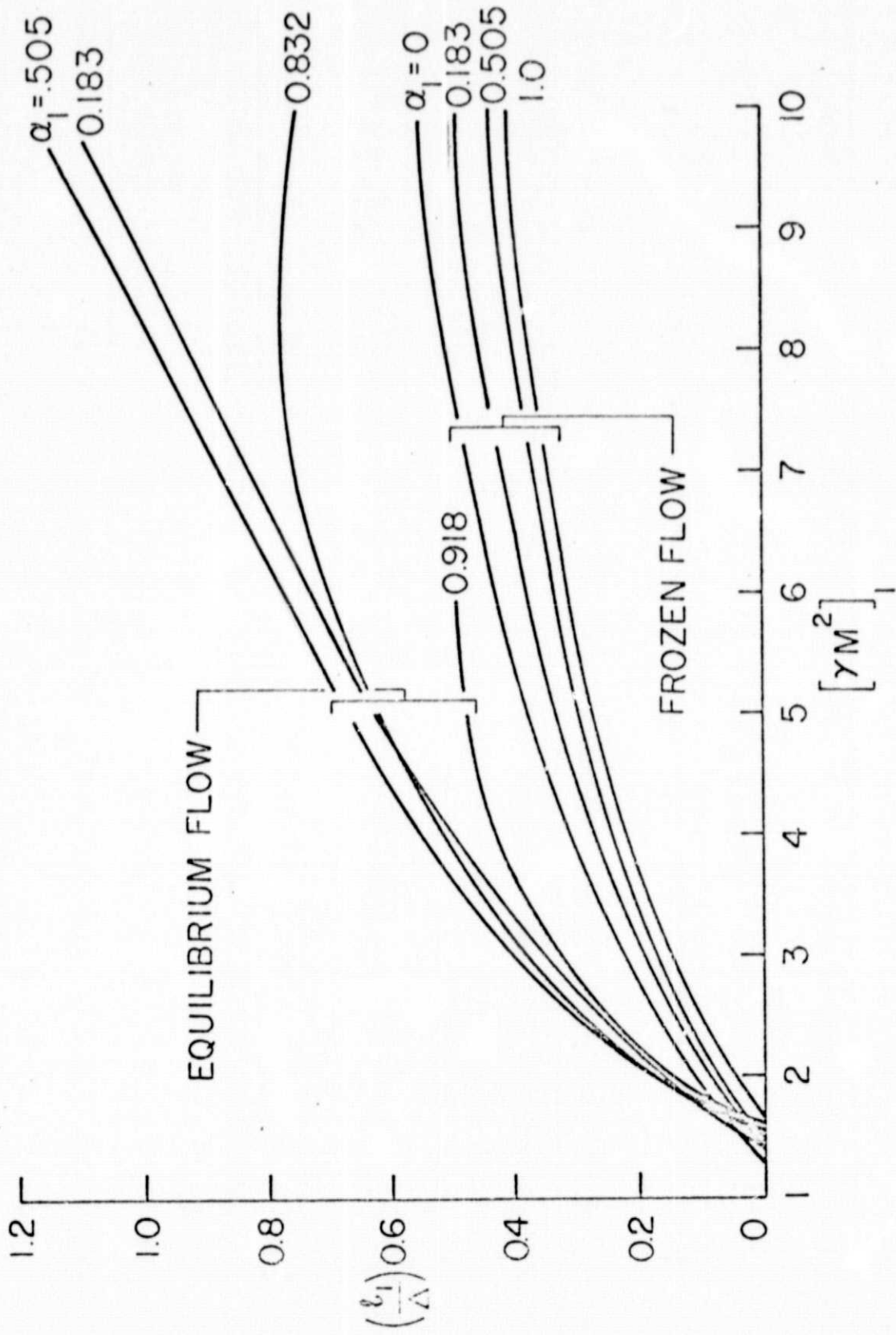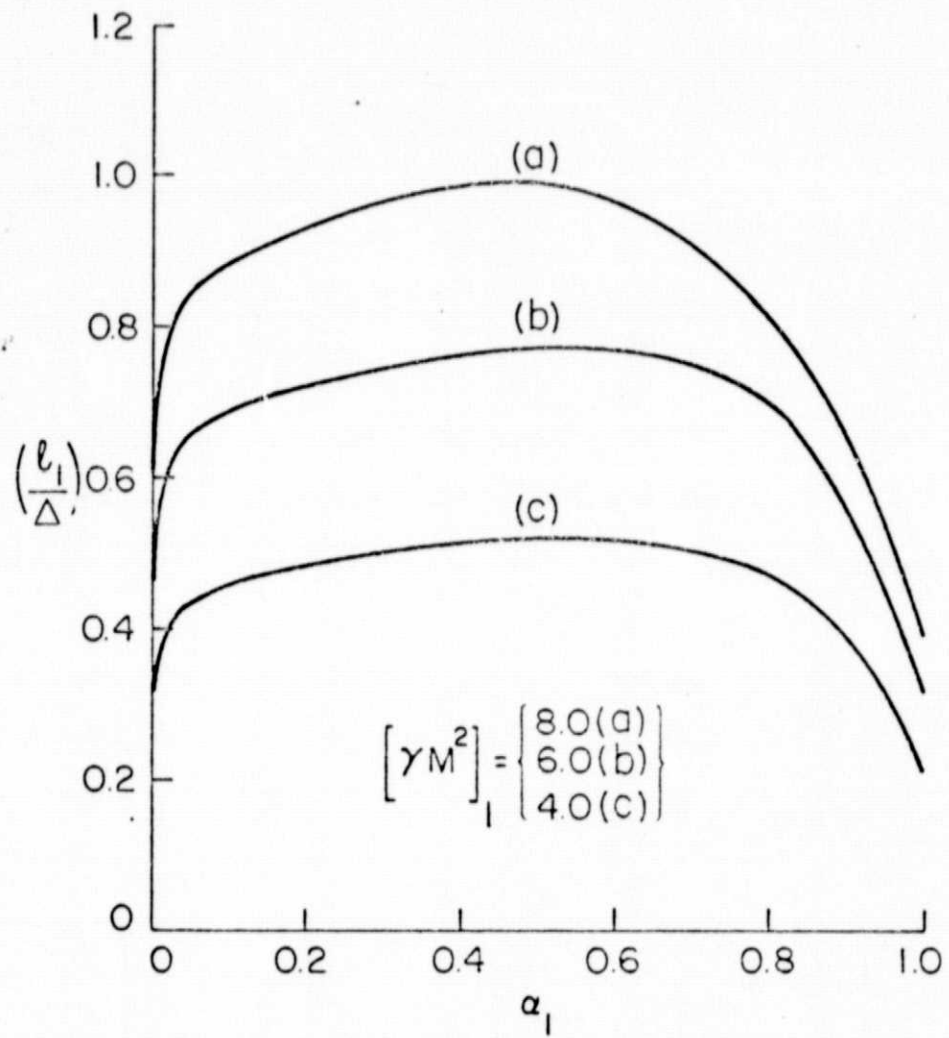
α/α_0

τ/τ_2

v/v_1

(X/L)
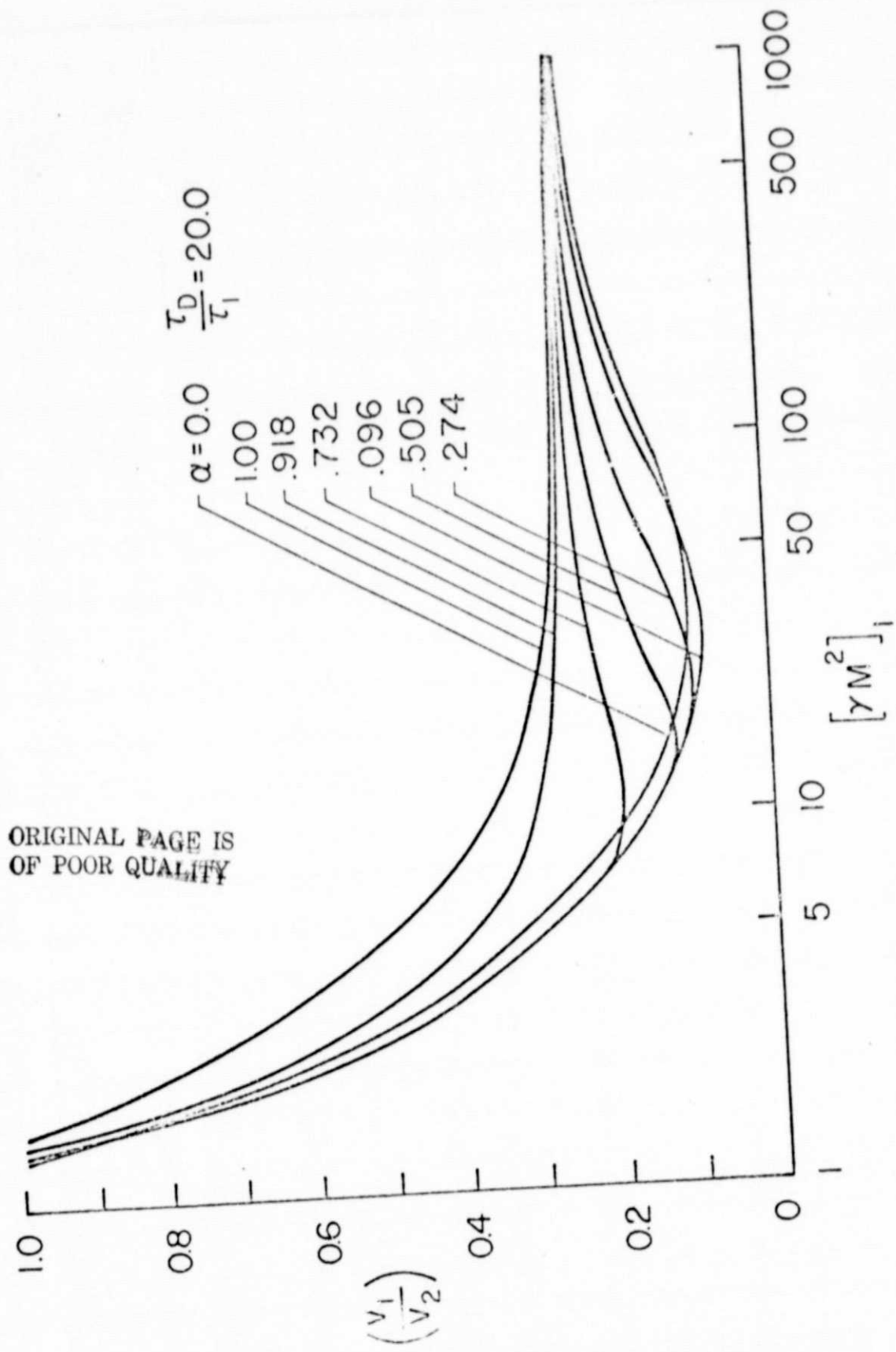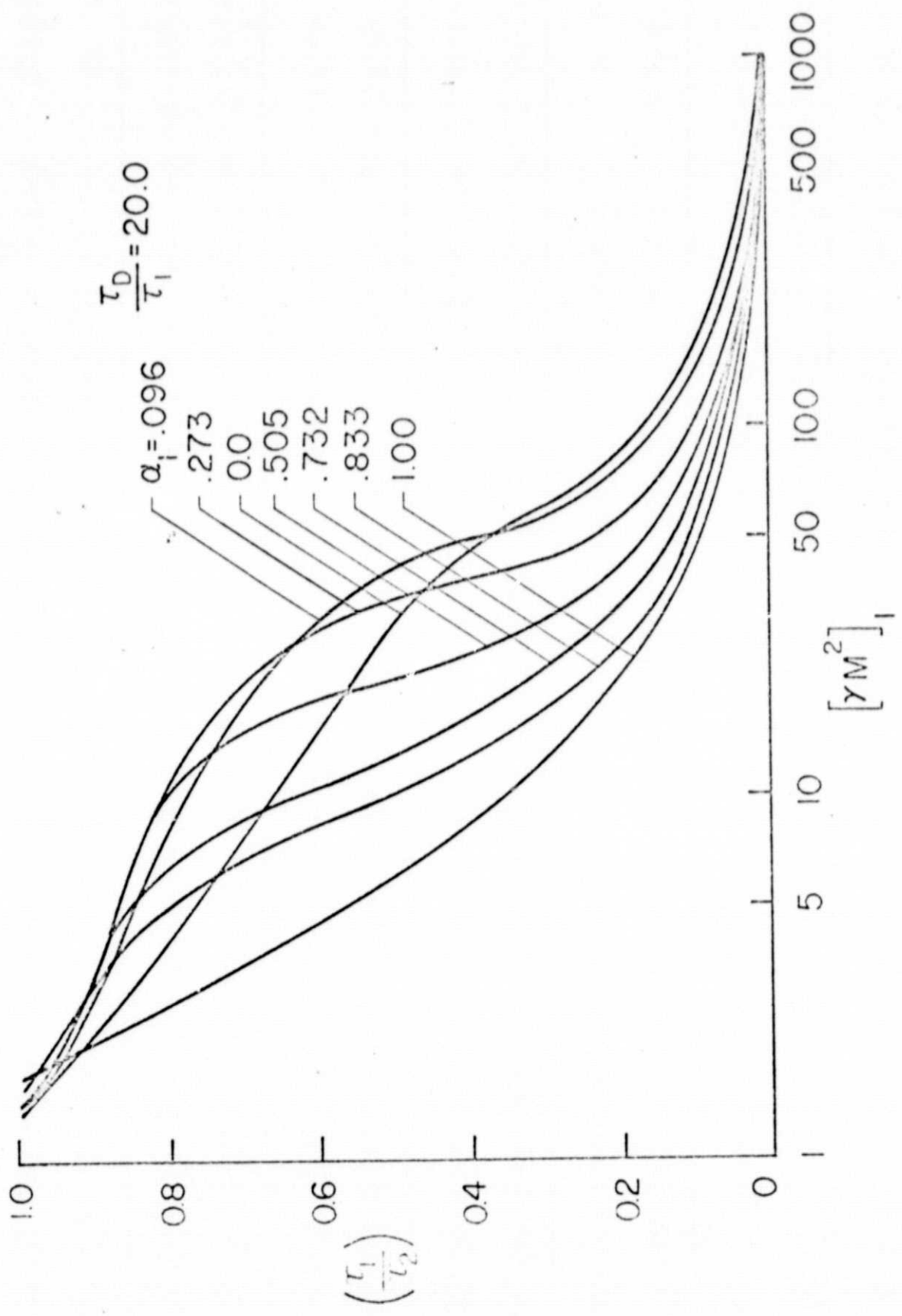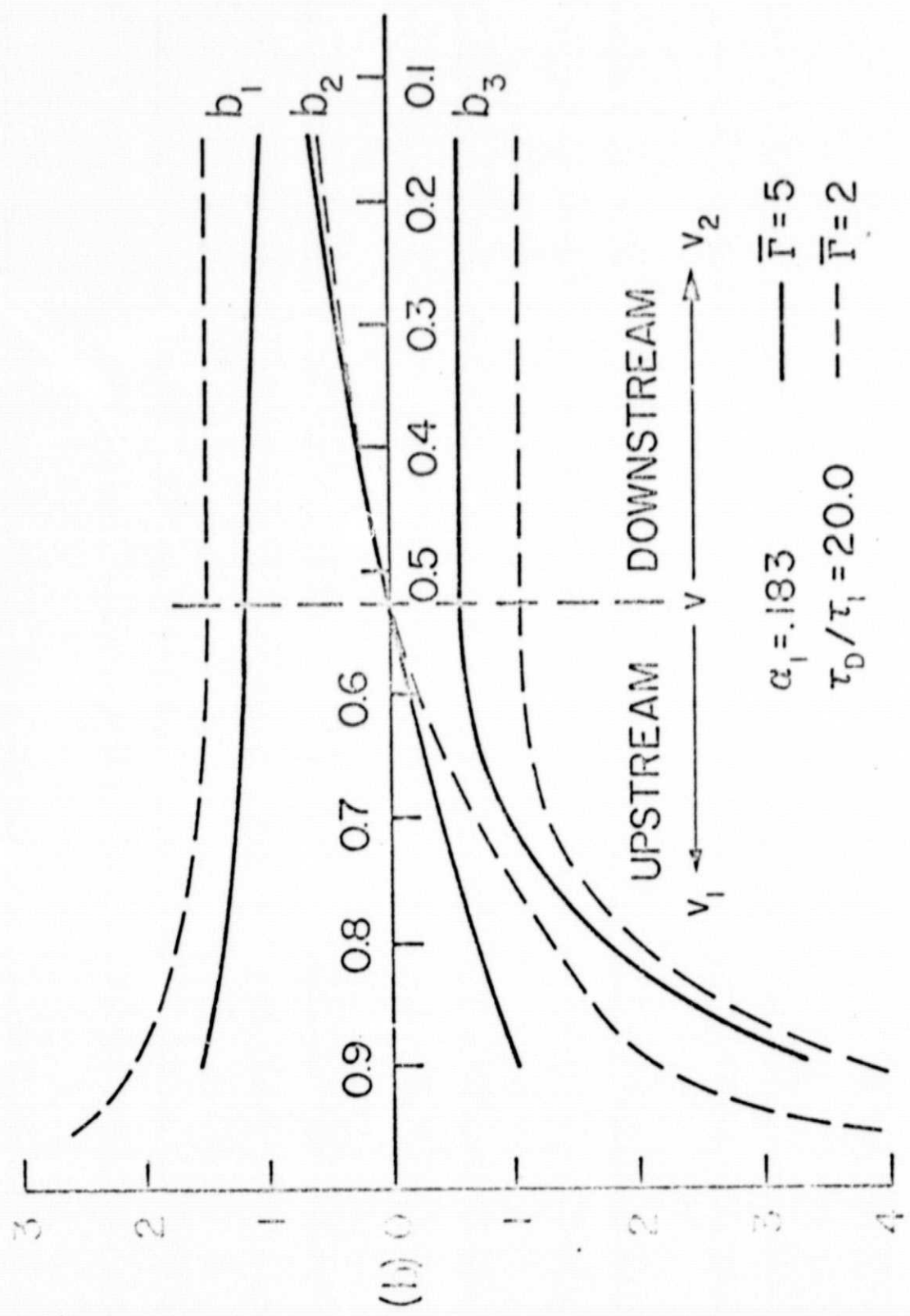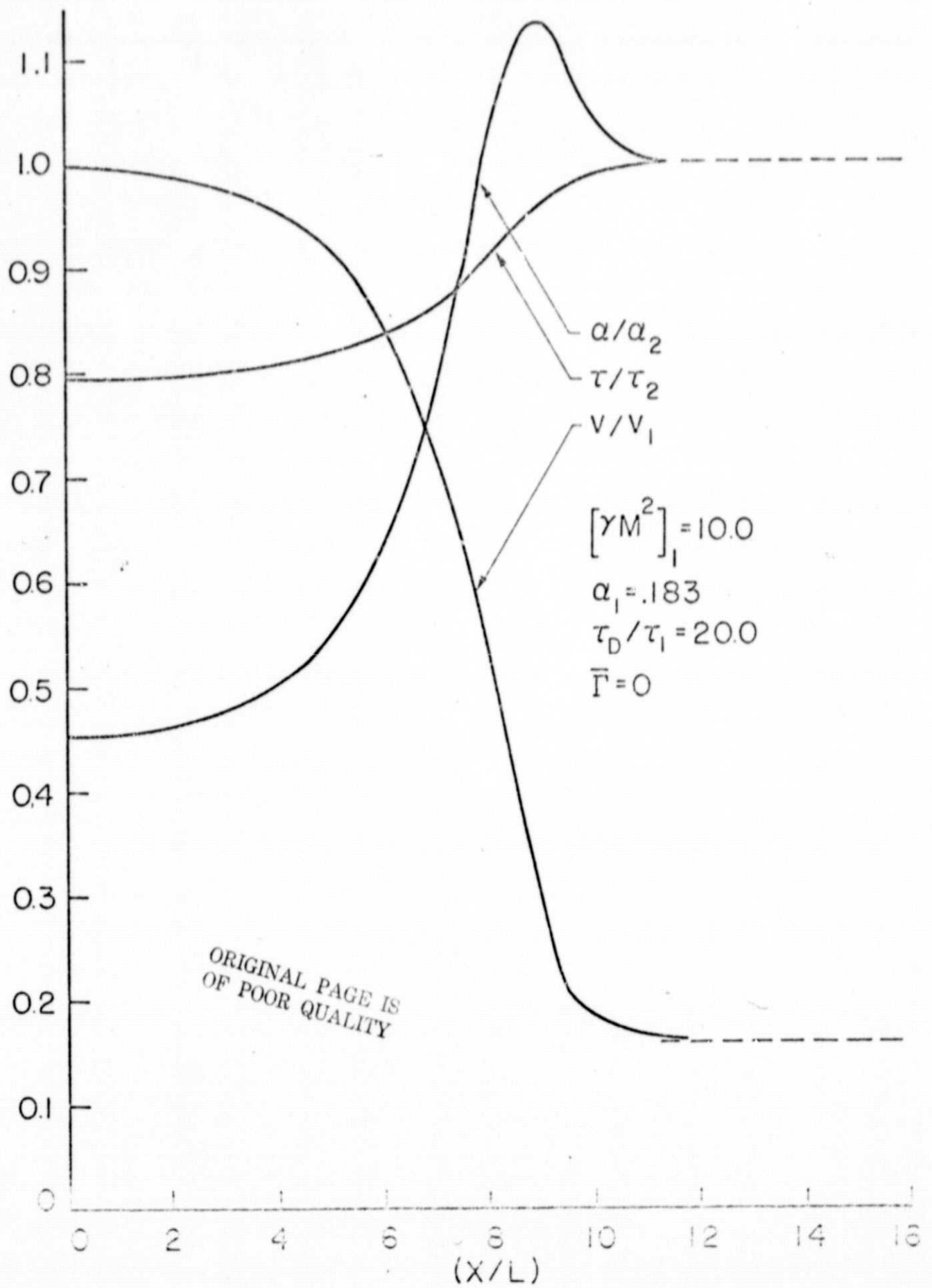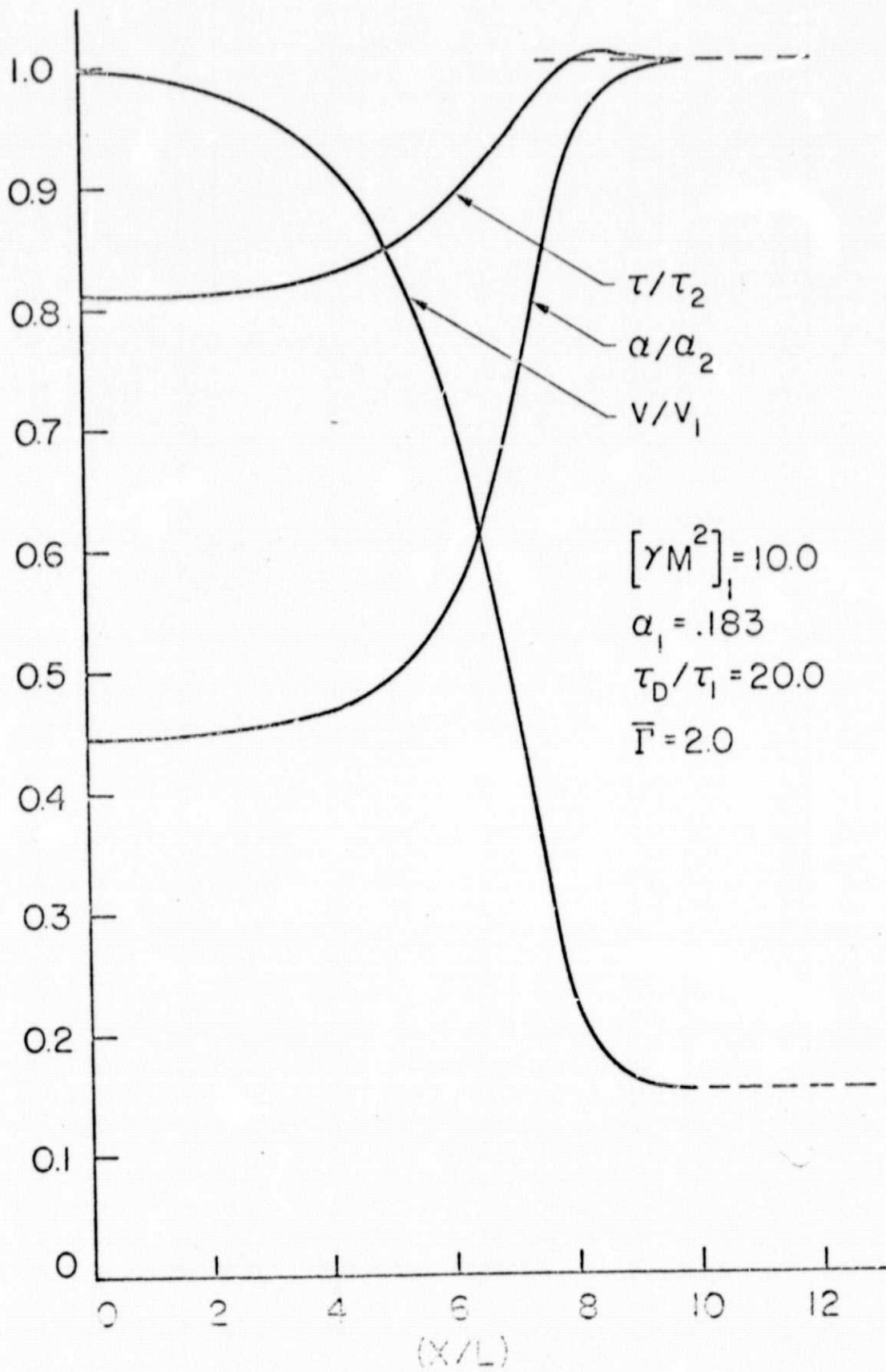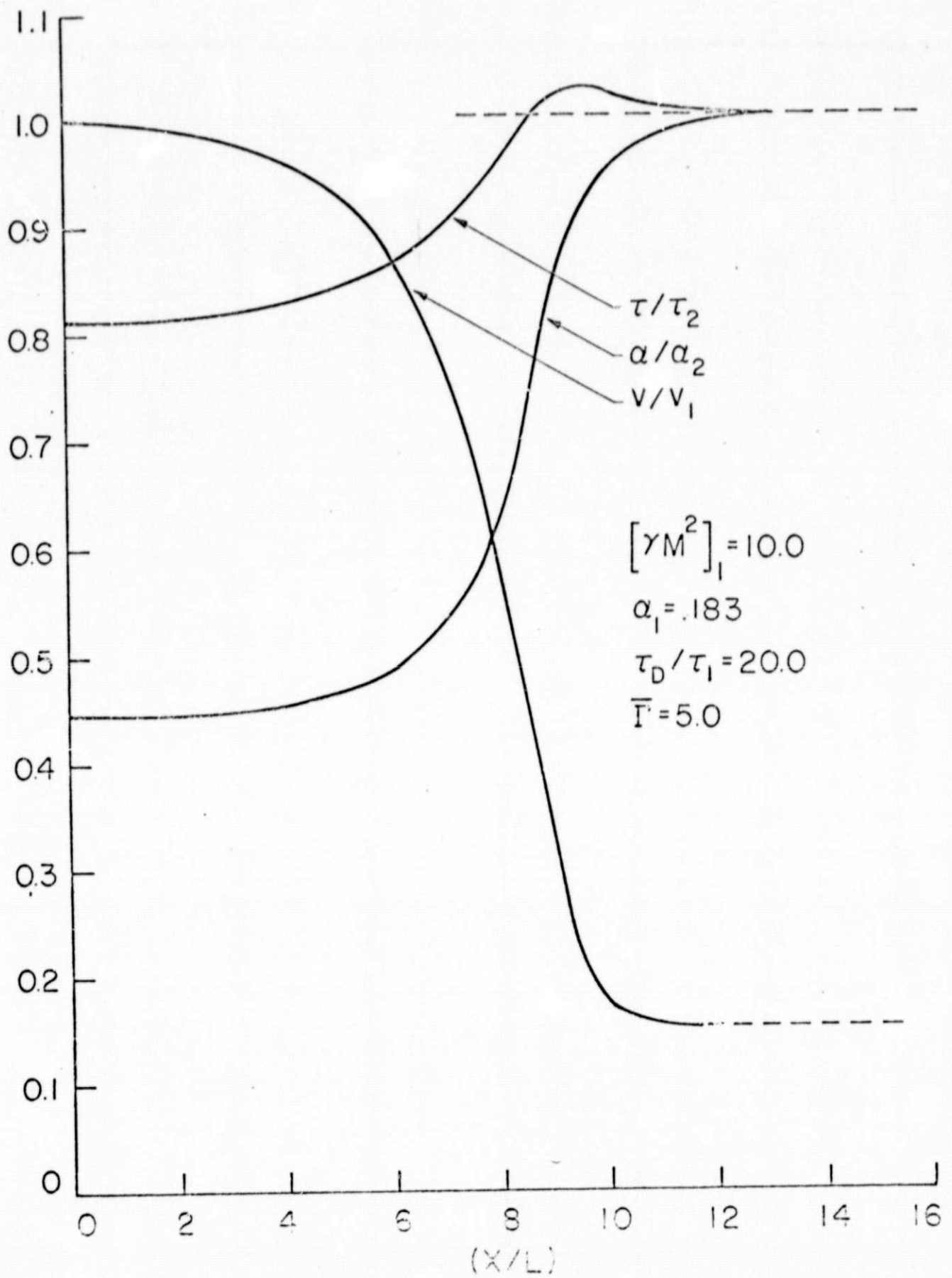
(a) THOMAS, $\mu \sim T^{\frac{1}{2}}$, $\gamma = 7/5$, $C_p \mu / \lambda = 3/4$ ⎤ PURE GAS

(b) MOTT–SMITH, KINETIC THEORY,
    $\gamma = 5/3$, $C_p \mu / \lambda = 2/3$ ⎦

(c) FROZEN, $\alpha_1 = 0.0$ ⎤
(d) FROZEN, $\alpha_1 = 1.0$ ⎦ PRESENT ANALYSIS
(e) EQUILIBRIUM, $\alpha_1 = .832$ ⎦

Axes: $\left(\dfrac{\ell_1}{\Delta} \right)$ versus $[\gamma M^2]_1$

$$\Delta_f = \frac{\left| f_1 - f_2 \right|}{\left| \dfrac{df}{d\left(\frac{x}{L}\right)} \right|_{max}}$$

$\alpha_1 = .18366$

$\left. \begin{array}{l} f = \tau \\ f = v \end{array} \right\}$ FROZEN FLOW

$\left. \begin{array}{l} f = \alpha \\ f = \tau \\ f = v \end{array} \right\}$ EQUILIBRIUM FLOW