

INFORMATION TO USERS

This material was produced from a microfilm copy of the original document. While the most advanced technological means to photograph and reproduce this document have been used, the quality is heavily dependent upon the quality of the original submitted.

The following explanation of techniques is provided to help you understand markings or patterns which may appear on this reproduction.

1. The sign or "target" for pages apparently lacking from the document photographed is "Missing Page(s)". If it was possible to obtain the missing page(s) or section, they are spliced into the film along with adjacent pages. This may have necessitated cutting thru an image and duplicating adjacent pages to insure you complete continuity.
2. When an image on the film is obliterated with a large round black mark, it is an indication that the photographer suspected that the copy may have moved during exposure and thus cause a blurred image. You will find a good image of the page in the adjacent frame.
3. When a map, drawing or chart, etc., was part of the material being photographed the photographer followed a definite method in "sectioning" the material. It is customary to begin photoing at the upper left hand corner of a large sheet and to continue photoing from left to right in equal sections with a small overlap. If necessary, sectioning is continued again — beginning below the first row and continuing on until complete.
4. The majority of users indicate that the textual content is of greatest value, however, a somewhat higher quality reproduction could be made from "photographs" if essential to the understanding of the dissertation. Silver prints of "photographs" may be ordered at additional charge by writing the Order Department, giving the catalog number, title, author and specific pages you wish reproduced.
5. PLEASE NOTE: Some pages may have indistinct print. Filmed as received.

University Microfilms International

300 North Zeeb Road
Ann Arbor, Michigan 48106 USA
St. John's Road, Tyler's Green
High Wycombe, Bucks, England HP10 8HR

7817885

HSEU, JIN-SHOU HAMILTON
COMBUSTION WAVES ASSOCIATED WITH WEAK
DISTURBANCES.

THE UNIVERSITY OF OKLAHOMA, PH.D., 1977

University
Microfilms
International 300 N ZEEB ROAD, ANN ARBOR, MI 48106

UNIVERSITY OF OKLAHOMA
GRADUATE COLLEGE

COMBUSTION WAVES ASSOCIATED WITH WEAK DISTURBANCES

A THESIS
SUBMITTED TO THE GRADUATE FACULTY
in partial fulfillment of the requirements for the
degree of
DOCTOR OF PHILOSOPHY

By
JIN-SHOU HAMILTON HSEU
Norman, Oklahoma
1977

COMBUSTION WAVES ASSOCIATED WITH WEAK DISTURBANCES

A THESIS

APPROVED FOR THE SCHOOL OF AEROSPACE, MECHANICAL,
AND NUCLEAR ENGINEERING

By

Maurice Rasmussen

Martin C. Ischke

John E. Francis

C. M. Stepanick

E. J. Block

TABLE OF CONTENTS

	Page
ACKNOWLEDGMENT	iii
ABSTRACT	iv
NOMENCLATURE	vi
LIST OF ILLUSTRATIONS.	x
 Chapter	
I. INTRODUCTION	1
II. FORMULATION OF THE PROBLEM	
2.1 Governing Equations	5
2.2 Linearized Theory	9
2.3 Reduced Equations	14
2.4 Solution by Laplace Transformation.	20
2.5 Laminar Flame Propagation	23
2.6 Equilibrium Speed of Sound.	29
III. APPLICATION TO HOT-SURFACE IGNITION OF GASES	
3.1 Statement of the Problem.	33
3.2 Laplace-Transform Analysis	35
3.3 Ignition at a Constant Surface	
Temperature	39
3.4 Ignition by a Constant Heat Flow.	51
IV. APPLICATION TO EXPLOSION PROBLEM	
4.1 Description of the Problem.	58

Table of Contents (Cont'd.)

	Page
4.2 Laplace-Transform Analysis	60
4.3 Asymptotic Approximation for Large Time	64
V. NONLINEAR INTERACTION	69
VI. CONCLUDING REMARKS.	77
REFERENCES.	79
APPENDIX	
A. SEVENTH-ORDER PARTIAL DIFFERENTIAL EQUATION FOR THE VELOCITY POTENTIAL	84

ACKNOWLEDGMENTS

The author wishes to express his deep indebtedness and appreciation to his advisor, Dr. Maurice L. Rasmussen, for his guidance, encouragement, and assistance throughout this work. Thanks are due also to all members of the authors' graduate committee, Dr. E.F. Blick, Dr. J.E. Francis, Dr. M.C. Jischke, and Dr. C.M. Sliepcevich, for their interest and criticism in this work. The author also wishes to thank Dr. S.R. Gollahalli for his enthusiasm and help.

To my wife Jean, for her patience and understanding, I will always be grateful. The excellent job of typing by Shirley Ray is appreciated. Also, I am grateful for the financial assistance offered by the School of Aerospace, Mechanical, and Nuclear Engineering in the course of my study.

ABSTRACT

A theoretical investigation is focused on the combined effects of gas dynamics, viscosity, heat conduction, mass diffusion, and chemical reactions on the wave propagation induced by weak disturbances. The governing equations for multicomponent reacting gas mixtures are set up within the framework of a general linearized theory. The combustion process is approximated by a simple one-step reaction involving a ternary mixture of oxidant, fuel, and product. The pertinent governing partial differential equation for the velocity potential is derived and applied to several specific physical problems. Laplace transform techniques are utilized to obtain asymptotic long-time wave behavior. It has been shown that Burgers' equation is the appropriate description of the equilibrium wave propagation. A general expression for the laminar flame speed which displays the dependency on the reaction order, heat of combustion, characteristic reaction time, and the transport properties of the system is obtained in the study.

The theory is demonstrated by two basic problems: a hot-surface ignition problem and a one-dimensional explosion problem, that is, the shock-tube problem. The associated

complex processes are illustrated and interpreted by explicit asymptotic solutions. The induced temperature, pressure, velocity, and species concentration disturbances for the reacting mixture are plotted and discussed, particularly with regard to the wave disturbances.

NOMENCLATURE

a_e, a_f	Equilibrium and frozen sound speeds, respectively
A	Preexponential factor
b_e, b_w	Factors of diffusive spreading; defined in equation (2.4.8)
C_p	Frozen specific heat at constant pressure
$C_{p,\alpha}$	Specific heat of α at constant pressure
C_w	Dimensionless speed of laminar flame (deflagration wave)
D	Binary diffusion coefficient
$\bar{D}_{\alpha\beta}$	Multi-component diffusion coefficient
$D_{\alpha}^{(p)}$	Pressure diffusion coefficient
E_A	Activation energy for the reaction
E_Q	Energy liberated by the reaction
f	Stoichiometric coefficient for fuel species
g	Stoichiometric coefficient for product species
h	Enthalpy
h_{α}°	Enthalpy of formation of species α
\vec{j}_{α}	Diffusion-flux vector for species α
K_{α}	Chemical rate of production per unit mass for species α

$K(T, \rho)$	Equilibrium constant for the reaction
k	Thermal conductivity
k_α	Dimensionless pressure-diffusion coefficient
L_e	Lewis number
P	Pressure
P_r	Effective Prandtl number
\vec{q}	Heat-flux vector
Q	Dimensionless effective heat of reaction
R_α	Specific gas constant for species α
R	Rate of progress of the reaction
\hat{R}	Linearized rate of reaction function
\vec{r}	Dimensionless position vector
\vec{r}	Dimensional position vector
S_c	Effective Schmidt number
s	Laplace transform variable
T	Temperature
t	Time
u	Velocity component in x direction
\vec{V}	Velocity vector
\bar{W}	Average molecular weight of the mixture
W_α	Molecular weight of species α
X	Stretched coordinate defined in (5.1.23)

x	Dimensionless one-dimensional spatial coordinate
Y_α	Mass fraction of species α
$\Gamma(\eta)$	Gamma function
γ	Effective ratio of specific heats
δ	Dimensionless multi-diffusion coefficient
Δ	Mixture strength parameter ($\equiv \Delta_F - \sigma \Delta_X$)
$\Delta_A, A=\rho, T, P---$	Initial differential of various state variables across the diaphragm
Δ_T	Temperature jump on the hot-surface
$\dot{\epsilon}$	Rate of strain tensor
ϵ	Small perturbation parameter
ζ_w	Damping factor
η	Stretched spatial coordinate, defined in equation (5.1.26)
κ	Boltzmann's constant
λ	Second coefficient of viscosity
μ	First coefficient of viscosity
ν^*	Diffusivity factor, defined in equation (5.1.27)
ξ	Stretched coordinate, defined in equation (5.1.23)
ρ	Density
σ	Stoichiometric mass ratio ($\equiv fW_F / \chi W_X$)
$\dot{\tau}$	Viscous stress tensor
τ	Nondimensional time
τ_f	Characteristic forward chemical reaction time

τ_r	Characteristic reverse chemical reaction time
τ_f^*	Damkohler's second similarity group
ϕ	Velocity potential
$\bar{\phi}$	Laplace transform of ϕ
χ	Stoichiometric coefficient for oxidant species
∇^2	Laplacian operator
$()_0$	Variable evaluated at ambient conditions
$()'$	Perturbation quantity
\sim	Asymptotically equal to (in some given limit)

LIST OF ILLUSTRATIONS

Figure		Page
2.1	Variation of Non-dimensional Laminar Flame Speed with Second Damkohler Similarity Group	27
3.1	Diffusive Wave Behavior of Function $I(x, \tau; b, C)$	41
3.2	Long-time Behavior of the Temperature Perturbation for Ignition of Gases at a Constant Surface Temperature	45
3.3	Long-time Behavior of the Velocity Per- turbation for Ignition of Gases at a Constant Surface Temperature	48
3.4	Long-time Behavior of the Species Con- centration of Oxidant for Ignition of Gases at a Constant Surface Temperature.	49
3.5	Diffusive Wave Behavior of Function $U(x, \tau; b, C)$	53
3.6	Long-time Behavior of the Temperature Perturbation for Ignition of Gases by a Constant Heat Flow	54
3.7	Long-time Behavior of the Velocity Per- turbation for Ignition of Gases by a Constant Heat Flow	55
3.8	Long-time Behavior of the Species Con- centration of Oxidant for Ignition of Gases by a Constant Heat Flow.	56
4.1	Configuration for One-dimensional Explosion Problem.	58, 59

CHAPTER I

INTRODUCTION

Combustion phenomena can be categorized as involving either a homogeneous mixture of reactants combined before ignition occurs, or a reaction between initially unmixed reactants that meet at the flame. The non-premixed combustion, such as the burning of gaseous fuel jet, a carbon sphere, and a candle, is conventionally termed a diffusion flame, since the mixing of fuel and oxidizer must be accomplished by a diffusion process. In the premixed situation, exemplified by a Bunsen burner with primary air entrainment and by flames in a gasoline engine, combustion is localized near wave fronts associated with nonequilibrium and diffusive processes. These can be subdivided into detonation and deflagration types of waves. In different practical situations, all these types of combustion are encountered.

To describe the combustion problem rigorously, the equation of continuity, the equation of motion, the energy equation, the diffusion equation, and the equation of state must be set up, including chemical-reaction and heat-generation terms, in the appropriate coordinate system and with the initial and boundary conditions. Unfortunately, owing to the nonlinearity

and complexity of the equations, complete analytic solutions appear impossible. There are various approaches for obtaining solutions to the governing equations of combustion dynamics. Among many numerical schemes are the notable methods of Friedman and Burke [1], Spalding, Stephenson, and Taylor [2], Bledjian [3], Vance and Krier [4], and Smoot, Hieker, and Williams [5], among others. Numerical results can give precise numbers, but they usually are for restrictive situations and leave the interplay of the pertinent parameters obscure. As recommended in the review article of Williams[6], considerable insight into combustion problems can be obtained by considering the limit of large activation energy. The notion of activation energy asymptotics has been exploited by Bush and Fendell[7], Berman and Riazantsev [8], and Clarke [9] in their analysis of plane deflagration waves. The idea was also taken up by Williams [10], Ludford[11], and Buckmaster, Kapila, and Ludford [12] in connection with problems of heterogeneous combustion between solid and gas. A much more general asymptotic analysis in flame theory has been derived and reviewed by Clarke [13]. A third approach which can complement the previous two is that of linearized theory.

When the external disturbances are small, it is expected that the responses of the flow field are also small perturbations from the ambient conditions. Consequently, as a first-order approximation, the governing equations can be linearized. Then the analysis is simplified enough to allow

one to carry out a unified discussion of the various effects. It has been known for a long time that linearized theory is a mainstay in fluid mechanics problems. It provides not only the over-all picture, but also important insights into the features of the exact nonlinear problems. A linearized theory involving a diffusion flame in steady flow has been developed by Clarke [14,15]. A corresponding theory involving diffusion flames associated with weak explosions has been studied by Rasmussen [16,17,18]. A linearized theory for duct flows with combustion has been utilized by Williams [19]. The viewpoint of linearized analysis has also been employed previously by Moore and Curtis [20] and Sforza and Bloom [21] to study nonequilibrium dissociating gas flow. It is the purpose of the present paper to apply this well-known technique of linearization to the study of a class of problems.

Specifically, the following two problems are to be considered in the investigation: A. A semi-infinite region filled with a reacting gas mixture, initially in equilibrium, is disturbed by an impulsive temperature increase at the boundary end wall, and the consequent response to the action is to be studied. This problem is associated with the ignition of a combustible gas in contact with a heated wall. B. Initially two mixtures are separated by diaphragm. Across the diaphragm, small differences in pressure, temperature, and chemical composition exist. At a given instant, the diaphragm is removed, and the subsequent

flow is to be determined. This applies to situations where bubbles of hot burned gas are injected into a medium of fuel gas mixture. The problems envisaged here are inherently unsteady and involve propagation of various waves arising from thermal and mass diffusive mixing, chemical heat release, and nonequilibrium changes of state.

In the following analysis, we start the formulation with the linearization of the governing equations for a multi-component reacting ideal gas mixture based on the small-perturbation model which includes a linearized reaction rate. Pressure diffusion and multicomponent diffusion are included. Moreover, attention is confined to the general one-step reversible reaction represented by $\{\text{Fuel}\} + \{\text{Oxidant}\} = \{\text{Product}\}$. The linearized equations are manipulated so that a single ninth-order partial differential equation for the velocity potential is derived and applied to case A listed above. For case B, a simpler analysis employs Fick's law of diffusion and results in a similar governing equation which is of seventh-order. Solutions are obtained by means of the Laplace-transform technique. Asymptotic solutions valid for large times, which are the regime of interest, are obtained by the method of Rasmussen [22]. Some interesting features demonstrated by the exemplary problems are deduced and compared with existing results where possible. Finally, some effects of nonlinearities on the equilibrium wave front are demonstrated by showing that the one-dimensional wave front is governed by the well-known Burgers' equation.

CHAPTER II

FORMULATION OF THE PROBLEM

2.1 Governing Equations

The equations of conservation of mass, species, momentum, and energy for the ternary system of reacting species are (with body forces neglected)

$$\frac{D\rho}{Dt} + \rho \operatorname{div} \vec{V} = 0 \quad (2.1.1)$$

$$\rho \frac{DY_\alpha}{Dt} = - \operatorname{div} \vec{j}_\alpha + \rho K_\alpha, \quad \alpha = X, F, P \quad (2.1.2)$$

$$\rho \frac{D\vec{V}}{Dt} = - \operatorname{grad} P + \operatorname{div} \vec{\tau} \quad (2.1.3)$$

$$\rho \frac{Dh}{Dt} = \frac{DP}{Dt} + \vec{\tau} : \vec{\epsilon} - \operatorname{div} \vec{q} \quad (2.1.4)$$

where ρ is the mass density, \vec{V} the mass mean velocity, Y_α the mass fraction of species α , \vec{j}_α the diffusion-flux vector for species α , K_α the mass rate of production of species α per unit mass, P the pressure, $\vec{\tau}$ the viscous stress tensor, h the enthalpy, $\vec{\epsilon}$ the rate of strain tensor, and \vec{q} the heat flux vector. We assume the stress and the rate of strain are related by the Navier-Stokes relations

$$\vec{\tau} = 2\mu\vec{\epsilon} + \lambda(\text{div } \vec{V}) \vec{I} \quad (2.1.5)$$

$$\vec{\epsilon} = (1/2) [\nabla\vec{V} + (\nabla\vec{V})^t] \quad (2.1.6)$$

where μ and λ are the first and second coefficient of viscosity. The diffusion-flux and heat-flux vectors are given by

$$\vec{j}_X = - \tilde{D}_{11} \nabla Y_X - \tilde{D}_{12} \nabla Y_F - D_X^{(p)} \nabla \ln P \quad (2.1.7)$$

$$\vec{j}_F = - \tilde{D}_{21} \nabla Y_X - \tilde{D}_{22} \nabla Y_F - D_F^{(p)} \nabla \ln P \quad (2.1.8)$$

$$\vec{q} = - k\nabla T + (h_X - h_p) \vec{j}_X + (h_F - h_p) \vec{j}_F \quad (2.1.9)$$

if radiation, thermal diffusion, and the concomitant Dufour effect are neglected. These constitutive relations can be derived from kinetic theory [23] or by means of continuum mechanics [16]. Similar relations have also been developed by using the generalized Grad method [24], which is based on the expansion of the molecular velocity distribution functions of each of the components in a series in irreducible Hermitian tensor polynomials. The $\tilde{D}_{\alpha\beta}$ quantities are multicomponent diffusion coefficients and are functions of species mass fractions and binary diffusion coefficients. The pressure diffusion coefficient for species α is denoted by $D_\alpha^{(p)}$. The product terms Y_p , \vec{j}_p , and K_p satisfy the relations

$$Y_X + Y_F + Y_p = 1 \quad (2.1.10)$$

$$\vec{j}_X + \vec{j}_F + \vec{j}_p = 0 \quad (2.1.11)$$

$$K_X + K_F + K_p = 0 \quad (2.1.12)$$

The system is closed when the thermal and caloric equations of state of the form

$$P = P(\rho, T, Y_\alpha) \quad , \quad h = h(\rho, T, Y_\alpha) \quad (2.1.13)$$

are added, together with expressions for the mass rate of production for species α , K_α . If the individual gases are presumed to be thermally perfect, the thermal and caloric equations of state can be written in the forms

$$P = \rho T [(R_X - R_P) Y_X + (R_F - R_P) Y_F + R_P] \quad (2.1.14)$$

$$h = Y_X (h_X - h_P) + Y_F (h_F - h_P) + h_P \quad (2.1.15)$$

$$h_\alpha = \int_{T_0}^T C_{p,\alpha} dT + h_\alpha^0 \quad , \quad \alpha = X, F, \text{ or } P. \quad (2.1.16)$$

In the above, R_X , R_F , R_P are the specific gas constants for the oxidant, fuel, and product species, $C_{p,\alpha}$ the specific heat of α at constant pressure, and h_α^0 the enthalpy of formation of species α .

Equations (2.1.15) and (2.1.16) can be combined to read

$$h = \int_{T_0}^T C_p dT + Y_X (h_X^0 - h_P^0) + Y_F (h_F^0 - h_P^0) + h_P^0 \quad (2.1.17)$$

where C_p is the frozen specific heat at constant pressure defined as

$$C_p = \left(\frac{\partial h}{\partial T} \right)_{P, Y_\alpha} = Y_X (C_{p,X} - C_{p,P}) + Y_F (C_{p,F} - C_{p,P}) + C_{p,P} \quad (2.1.18)$$

The combustion scheme in this study will be simplified by assuming that f fuel molecules (chemical symbol F) combine with χ oxidant molecules (X) to form g product molecules (P), that is,



For reaction (2.1.19) the mass rates of production are expressed as

$$\begin{aligned} K_X &= - \chi W_X R \\ K_F &= - f W_F R \end{aligned} \quad (2.1.20)$$

$$\begin{aligned} K_P &= g W_P R \\ R &= \frac{Y_X^\chi Y_F^f}{\tau_f} - \frac{Y_P^g}{\tau_r} \\ &= \frac{1}{\tau_f} \left(Y_X^\chi Y_F^f - K(T, \rho) Y_P^g \right) \end{aligned} \quad (2.1.21)$$

where W_α ($\alpha = X, F, P$) is the molecular weight of species α . The quantity R , is the rate of progress of the reaction and τ_f and τ_r are the relevant forward (reactant \rightarrow product) and reverse (product \rightarrow reactant) characteristic reaction times. We refer to the function

$$K(T, \rho) = \frac{\tau_f}{\tau_r} = B(\rho T)^{g-\chi-f} \exp\left\{-\frac{E_Q}{kT}\right\} \quad (2.1.22)$$

as the equilibrium constant for the reaction. The characteristic forward reaction time, τ_f , which is strongly temperature

dependent, is assumed to be given by the Arrhenius law:

$$\frac{1}{\tau_f} = A \left(\frac{\rho}{W_X} \right)^X \left(\frac{\rho}{W_F} \right)^F T^\alpha \exp \left(- \frac{E_A}{\kappa T} \right) \quad (2.1.23)$$

In the above, A, B, α , and κ are constants, E_Q is the energy liberated by the reaction, and E_A is the activation energy for the reaction. The Arrhenius factor $\exp(-E_A/\kappa T)$ is responsible for the fact that combustion process occurs only when the temperature T is comparable to or greater than the activation temperature E_A/κ , a given constant. It is this feature which makes combustion a highly temperature-dependent phenomenon.

2.2 Linearized Theory

The following analysis will be based on the theory of small perturbations. By small perturbations, we mean that the resulting flow fields induced by weak disturbances are small perturbations from the ambient condition. Then we may define dimensionless perturbation variables as follows:

$$\begin{aligned} \rho &= \rho_0 (1 + \rho') \\ P &= P_0 (1 + P') \\ T &= T_0 (1 + T') \\ Y_\alpha &= Y_{\alpha 0} + Y'_\alpha, \quad \alpha = X, F, P \\ \vec{V} &= a_{f0} \vec{V}' \end{aligned} \quad (2.2.1)$$

The primed symbols represent perturbations from the ambient state (subscript naught), where $|\rho'|, |P'|, |T'|, |Y'_\alpha| \ll 1$ every-

where, and $|\vec{V}| \ll a_{f_0}$, a_{f_0} being the frozen speed of sound in the uniform ambient state, defined as

$$a_{f_0}^2 = \gamma \frac{p_0}{\rho_0} \quad (2.2.2)$$

Here γ is the frozen specific heats ratio in the ambient state, defined as

$$\frac{\gamma-1}{\gamma} = \frac{(\sum R_\alpha Y_\alpha)_0}{(C_p)_0} \quad (2.2.3)$$

In general, the dissipative parameters $\mu, \lambda, k, \tilde{D}_{\alpha\beta}$, and $D_\alpha^{(p)}$ are functions of temperature. Again for simplicity we take them constant, since in the linearization only their leading terms (depending on T_0) will be involved.

The dimensionless time and space variables are now defined as

$$\tau \equiv \frac{\rho_0 a_{f_0}^2}{\tilde{\mu}_0} t, \quad \vec{r} = \frac{\rho_0 a_{f_0}}{\tilde{\mu}_0} \vec{r} \quad (2.2.4)$$

where $\tilde{\mu}_0 = 2\mu_0 + \lambda_0$ is the reduced viscosity and \vec{r} denotes the dimensional position vector.

Damkohler's second similarity group, the ratio of a characteristic chemical time to a characteristic molecular diffusion time, is then defined as

$$\tau_f^* \equiv \frac{\rho_0 a_{f_0}^2}{\tilde{\mu}_0} \tau_f$$

To further simplify the analysis it will be assumed that the multicomponent diffusion coefficients are related by

$$\hat{D}_{11} = \hat{D}_{22} \text{ and } \hat{D}_{12} = \hat{D}_{21} \quad (2.2.5)$$

With all of the foregoing assumptions the equations of 2.1 can be linearized by dropping all products and squares of perturbations. A set of linearized equations is obtained in the following form:

Continuity

$$\frac{\partial \rho}{\partial \tau} + \nabla \cdot \vec{V} = 0 \quad (2.2.6)$$

Species

$$D_S Y_X = \delta \nabla^2 Y_F + k_X \nabla^2 P - S_C X W_X \hat{R} \quad (2.2.7)$$

$$D_S Y_F = \delta \nabla^2 Y_X + k_F \nabla^2 P - S_C F W_F \hat{R} \quad (2.2.8)$$

Momentum

$$\frac{\partial \vec{V}}{\partial \tau} = - \frac{1}{\gamma} \nabla P + \nabla (\nabla \cdot \vec{V}) - \frac{\mu_0}{\mu_0} \nabla X (\nabla X \vec{V}) \quad (2.2.9)$$

Energy

$$D_P T = \frac{\gamma-1}{\gamma} P_r \frac{\partial P}{\partial \tau} + P_r Q \hat{R} \quad (2.2.10)$$

State

$$P = \rho + T + \alpha_X Y_X + \alpha_F Y_F \quad (2.2.11)$$

In these equations primes have been dropped with the understanding that all quantities are now dimensionless. Here ∇^2 is the dimensionless Laplacian operator and

$$D_S \equiv S_C \frac{\partial}{\partial \tau} - \nabla^2 \quad (2.2.12)$$

$$D_P \equiv P_r \frac{\partial}{\partial \tau} - \nabla^2$$

are the classical mass and thermal diffusion operators, $P_r = \tilde{\mu}_o C_p / k_o$ is the Prandtl number, $S_c = \tilde{\mu}_o / (D_{11})_o$ the Schmidt number, $\delta = (\tilde{D}_{12})_o / (\tilde{D}_{11})_o$ the nondimensional multi-diffusion coefficient, $k_\alpha = (D_\alpha^{(p)} / \tilde{D}_{11})_o$ the dimensionless pressure-diffusion coefficient for species α , and α_X and α_F defined as

$$\alpha_X \equiv \frac{R_X - R_p}{R_X Y_{X_o} + R_F Y_{F_o} + R_p Y_{p_o}} \quad (2.2.13)$$

$$\alpha_F \equiv \frac{R_F - R_p}{R_X Y_{X_o} + R_F Y_{F_o} + R_p Y_{p_o}}$$

The dimensionless effective heat of reaction, Q , appears in the energy equation (2.2.11), defined as

$$Q = \frac{\chi W_X (h_X - h_p)_o + f W_F (h_F - h_p)_o}{C_{p_o} T_o} \quad (2.2.14)$$

At this stage, it should be noted that the linearized equations in the set just referred to are coupled by the chemical rate terms since, in general, \hat{R} is a function of ρ , T , and the Y 's, as indicated by equation (2.1.21). Because of the a priori assumption that deviations from the ambient state of equilibrium are small, we shall assume that \hat{R} can be approximated from the linear terms of a multi-variate Taylor series, expanded about the uniform ambient state of equilibrium. Then the linearized rate of reaction function, \hat{R} , is given by

$$\begin{aligned} \hat{R} &= \hat{R}(\rho, T, Y_X, Y_F) \\ &= a_X Y_X + a_F Y_F - \beta_\rho \rho - \beta_T T \end{aligned} \quad (2.2.15)$$

where

$$\begin{aligned}
 a_X &= \frac{Y_{X_0}^X Y_{F_0}^f}{\tau_{f_0}^*} \left(\frac{\chi}{Y_{X_0}} + \frac{g}{Y_{P_0}} \right) \\
 a_F &= \frac{Y_{X_0}^X Y_{F_0}^f}{\tau_{f_0}^*} \left(\frac{f}{Y_{F_0}} + \frac{g}{Y_{P_0}} \right) \\
 \beta_\rho &= \frac{Y_{X_0}^X Y_{F_0}^f}{\tau_{f_0}^*} \left[\left(\frac{\partial \ln K}{\partial \ln \rho} \right)_T \right]_0 \\
 \beta_T &= \frac{Y_{X_0}^X Y_{F_0}^f}{\tau_{f_0}^*} \left[\left(\frac{\partial \ln K}{\partial \ln T} \right)_\rho \right]_0
 \end{aligned} \tag{2.2.16}$$

An expression for the logarithmic derivative of $K(T, \rho)$ with respect to temperature can be derived from the result in (2.1.22) in the form

$$\left[\left(\frac{\partial \ln K}{\partial \ln T} \right)_\rho \right]_0 = m + \frac{\gamma Q}{(\gamma - 1) \bar{W}} \tag{2.2.17}$$

where $m = g - \chi - f$ and $\bar{W} = \left[\Sigma \left(\frac{Y_\alpha}{W_\alpha} \right) \right]_0^{-1}$ is the average molecular weight of the mixture. Thus the temperature derivative of the equilibrium constant is given in terms of the effective energy of reaction, Q . The logarithmic derivative with respect to density is

$$\left[\left(\frac{\partial \ln K}{\partial \ln \rho} \right)_T \right]_0 = m \tag{2.2.18}$$

The density derivative at constant temperature is a constant.

The condition $\tilde{R} = 0$ denotes local thermodynamic equilibrium when $\tau_{f_0}^*$ vanishes but denotes frozen flow when $\tau_{f_0}^*$ becomes infinity. The functional form (2.2.15) is an extension of the simple non-equilibrium expressions discussed by Clarke and McChesney [25] and Vincenti and Kruger [26] in which only one non-equilibrium variable was contained. Here we have two non-equilibrium variables, Y_X and Y_F , pertaining to our simple ternary combustion model, equation (2.1.19).

2.3 Reduced Equations

The linearized problem can be simplified further by splitting the velocity vector into its irrotational and solenoidal parts [27]. The present study, however, is concerned with problems that are irrotational by virtue of planar symmetry; $\text{curl } \vec{V}$ vanishes identically. For these irrotational flows, we introduce the velocity potential such that

$$\vec{V} = \nabla \phi \quad (2.3.1)$$

The momentum equation (2.2.10) can now be integrated once and the pressure perturbation obtained as

$$P = \gamma (\nabla^2 \phi - \phi_\tau) \quad (2.3.2)$$

The time-function of integration has been set equal to zero since the pressure perturbation does not vary with time uniformly in space. The continuity equation (2.2.7) can now be written

$$\rho_{\tau} = - \nabla^2 \phi \quad (2.3.3)$$

Consider now the rate expression (2.2.16). Elimination of T by means of the thermal equation of state (2.2.12) yields

$$\dot{R} = A_X Y_X + A_F Y_F - \left[(\beta_{\rho} - \beta_T) \rho + \beta_T P \right] \quad (2.3.4)$$

where

$$A_X \equiv a_X + \alpha_X \beta_T \quad (2.3.5)$$

$$A_F \equiv a_F + \alpha_F \beta_T$$

Differentiation of \dot{R} with respect to time now yields

$$\ddot{R} = A_X Y_{X_{\tau}} + A_F Y_{F_{\tau}} - \phi(\phi) \quad (2.3.6)$$

where

$$\phi(\phi) = (\beta_T - \beta_{\rho}) \nabla^2 \phi + \gamma \beta_T (\nabla^2 \phi - \phi_{\tau})_{\tau} \quad (2.3.7)$$

with the aid of equations (2.3.2) and (2.3.3). The time derivative of the rate function now depends on the time derivatives of the mass fractions and the velocity potential. A single equation for the velocity potential can then be obtained by differentiating the energy equation (2.2.11) with time, eliminating the temperature T by means of equation (2.2.12), and utilizing equations (2.3.2) and (2.3.3) to eliminate P and ρ . We obtain

$$\begin{aligned} L(\phi) = & P_r Q \phi(\phi) - \{ \alpha_X D_p + P_r Q A_X \} Y_{X_{\tau}} \\ & - \{ \alpha_F D_p + P_r Q A_F \} Y_{F_{\tau}} \end{aligned} \quad (2.3.8)$$

where

$$\begin{aligned}
 L(\phi) &\equiv D_p(\rho_\tau - p_\tau) + \frac{\gamma-1}{\gamma} P_r P_{r\tau\tau} \\
 &\equiv \gamma \nabla^4 \phi_\tau + \nabla^2 \{ \nabla^2 \phi - (\gamma + P_r) \phi_{\tau\tau} \} + P_r (\phi_{\tau\tau} - \nabla^2 \phi)_\tau
 \end{aligned} \tag{2.3.9}$$

The effects of combustion and mass diffusion are contained in the terms on the right-hand side of equation (2.3.8).

By differentiating the diffusion equations (2.2.8) and (2.2.9) with respect to time, eliminating \dot{R}_τ by equation (2.3.6), we obtain two simultaneous equations for Y_X and Y_F .

$$\begin{aligned}
 (D_s + S_c \chi W_X A_X) Y_{X\tau} &= (\delta \nabla^2 - S_c \chi W_X A_F) Y_{F\tau} \\
 &\quad + K_X \nabla^2 P_\tau + S_c \chi W_X \phi(\phi)
 \end{aligned} \tag{2.3.10}$$

$$\begin{aligned}
 (D_s + S_c f W_F A_F) Y_{F\tau} &= (\delta \nabla^2 - S_c f W_F A_X) Y_{X\tau} \\
 &\quad + K_F \nabla^2 P_\tau + S_c f W_F \phi(\phi)
 \end{aligned} \tag{2.3.11}$$

Cross operation of the above equations yields the separate equations for Y_X and Y_F :

$$\begin{aligned}
 \Delta^4_{Y_{X\tau}} &= [k_X \{ D_s + S_c f W_F A_F \} + k_f \{ \delta \nabla^2 - S_c \chi W_X A_F \}] \nabla^2 P \\
 &\quad + S_c [\chi W_X D_s + f W_F \delta \nabla^2] \phi(\phi)
 \end{aligned} \tag{2.3.12}$$

$$\begin{aligned}
 \Delta^4_{Y_{F\tau}} &= [k_f \{ D_s + S_c \chi W_X A_X \} + k_X \{ \delta \nabla^2 - S_c f W_F A_X \}] \nabla^2 P \\
 &\quad + S_c [f W_F D_s + \chi W_X \delta \nabla^2] \phi(\phi)
 \end{aligned} \tag{2.3.13}$$

where the fourth-order operator Δ^4 is given by

$$\Delta^4 \equiv D_S^2 + S_C E_1 D_S - \delta^2 \nabla^4 + \delta S_C E_2 \nabla^2 \quad (2.3.14)$$

$$E_1 \equiv \chi W_X A_X + f W_f A_F \quad (2.3.15)$$

$$E_2 \equiv \chi W_X A_F + f W_f A_X$$

If we now operate on equation (2.3.8) with the operator Δ^4 and eliminate Y_X and Y_F by means of equations (2.3.12) and (2.3.13), a single equation for ϕ is obtained:

$$\begin{aligned} \Delta^4 L(\phi) = & [P_R Q \{D_S^2 - \delta^2 \nabla^4\} - S_C D_P \{E_3 D_S + E_4 \delta \nabla^2\}] \phi(\phi) \\ & - [D_P \{E_5 D_S + E_6 \delta \nabla^2\} + P_R Q \{E_7 D_S + E_8 \delta \nabla^2\} \\ & + S_C E_9 D_P] \nabla^2 P \end{aligned} \quad (2.3.16)$$

where

$$E_3 \equiv \chi W_X \alpha_X + f W_f \alpha_F$$

$$E_4 \equiv \chi W_X \alpha_F + f W_f \alpha_X$$

$$E_5 \equiv k_X \alpha_X + k_F \alpha_X$$

$$E_6 \equiv k_X \alpha_F + k_F \alpha_X \quad (2.3.17)$$

$$E_7 \equiv k_X A_X + k_F A_F$$

$$E_8 \equiv k_X A_F + k_F A_X$$

$$E_9 \equiv (\alpha_F A_X - \alpha_X A_F) (\chi W_X k_F - f W_f k_X)$$

Equation (2.3.16) can also be written as

$$\begin{aligned}
 & A_9 \nabla^8 \frac{\partial \phi}{\partial \tau} + \nabla^6 \left[(1 - \delta^2) \nabla^2 \phi - A_8 \frac{\partial^2 \phi}{\partial \tau^2} \right] - \nabla^4 \frac{\partial}{\partial \tau} \left[A_7 \nabla^2 \phi - B_7 \frac{\partial^2 \phi}{\partial \tau^2} \right] \\
 & - \nabla^2 \left[C_6 \nabla^4 \phi - A_6 \nabla^2 \frac{\partial^2 \phi}{\partial \tau^2} + B_6 \frac{\partial^4 \phi}{\partial \tau^4} \right] + \frac{\partial}{\partial \tau} \left[A_5 \nabla^4 \phi - B_5 \nabla^2 \frac{\partial^2 \phi}{\partial \tau^2} + P_r S_c^2 \frac{\partial^4 \phi}{\partial \tau^4} \right] \\
 & + A_4 \frac{\partial^2}{\partial \tau^2} \left[\frac{\partial^2 \phi}{\partial \tau^2} - C_e^2 \nabla^2 \phi \right] = 0 \tag{2.3.18}
 \end{aligned}$$

where

$$A_9 = \gamma \left[(1 - \delta^2) + E_5 - \delta E_6 \right]$$

$$A_8 = (1 - \delta^2) (\gamma + P_r) + \gamma \left[S_c (2 + E_5) + (E_5 - \delta E_6) (1 + P_r) \right]$$

$$\begin{aligned}
 A_7 = P_r (1 - \delta^2) + 2S_c + \gamma \left[S_c (E_1 - \delta E_2) + P_r Q (E_7 - \delta E_8) + S_c E_9 \right. \\
 \left. + \beta_T \left[P_r Q (1 - \delta^2) - S_c (E_3 - \delta E_4) \right] \right]
 \end{aligned}$$

$$B_7 = P_r (1 - \delta^2) + 2S_c (\gamma + P_r) + \gamma \left[S_c^2 + S_c E_5 (1 + P_r) + P_r (E_5 - \delta E_6) \right]$$

$$\begin{aligned}
 A_6 = 2S_c P_r + S_c (E_1 - \delta E_2) (\gamma + P_r) + S_c^2 (1 + \gamma E_1) \\
 + \gamma \beta_T \left[P_r Q (1 - \delta^2) - S_c \left[(E_3 - \delta E_4) (1 + P_r) - 2P_r Q + S_c E_3 \right] \right] \\
 + \gamma \left[P_r Q (E_7 - \delta E_8 + S_c E_7) + S_c E_9 (1 + P_r) \right]
 \end{aligned}$$

$$B_6 = S_c \left[P_r (2 + \gamma E_5) + S_c (\gamma + P_r) \right]$$

$$C_6 = S_c (E_1 - \delta E_2) + (\beta_T - \beta_\rho) \left[P_r Q (1 - \delta^2) - S_c (E_3 - \delta E_4) \right]$$

$$A_5 = S_c \left[P_r (E_1 - \delta E_2) + S_c E_1 - (\beta_T - \beta_\rho) \left[P_r (E_3 - \delta E_4) + E_3 S_c - 2P_r Q \right] \right]$$

$$\begin{aligned}
 B_5 = S_c \left[P_r (E_1 - \delta E_2) + P_r S_c + S_c E_1 (\gamma + P_r) + \gamma P_r (Q E_7 + E_9) \right. \\
 \left. + \gamma \beta_T \left[2P_r Q + P_r S_c (Q - E_3) - P_r (E_3 - \delta E_4) - S_c E_3 \right] \right]
 \end{aligned}$$

$$A_4 = P_r S_c^2 \left[E_1 + \gamma \beta_T (Q - E_3) \right]$$

$$C_e^2 = \frac{E_1 + (\beta_T - \beta_\rho) (Q - E_3)}{E_1 + \gamma \beta_T (Q - E_3)} \quad (2.3.19)$$

Equation (2.3.18) is the key equation in the present investigation, which is an extension of the linear wave equations studied extensively by Lick [28] and Whitham [29,30]. It is readily seen that this equation is a ninth-order partial differential equation, the highest-order term involving eight space derivatives and one time derivative. The last two terms in the equation are the lowest order terms and are related to the classical wave equation associated with inviscid acoustics. The higher-order terms reveal the combined effects due to viscosity, heat-conduction, mass-diffusion, and chemical reaction. To simplify the analysis and presentation the assumption of $\delta = k_X = k_F = 0$ will be made throughout the subsequent applications. In this case mass diffusion is adequately described in term of Fick's law, this means that

$$\vec{j}_\alpha = - \rho D \nabla Y_\alpha$$

where D is the binary diffusion coefficient. However, these parameters are retained here for further extension later on to assess the effects of pressure diffusion and multi-component diffusion.

2.4 Solution by Laplace Transformation

The Laplace transform with respect to t of a function $f(r,t)$ is defined as

$$L[f(r,t)] = \bar{f}(r,s) = \int_0^{\infty} e^{-st} f(r,t) dt \quad (2.4.1)$$

where s is the transform variable. Application of the transformation (2.4.1) to equation (2.3.18) yields an eight-order ordinary differential equation in the space variable. The assumed form $\bar{\phi}(x,s) = \exp(\lambda x)$ for the complimentary solution of the transformed equation leads to the characteristic equation for λ :

$$\begin{aligned} \lambda^8 [1 - \delta^2 + sA_9] - \lambda^6 [C_6 + sA_7 + s^2A_8] + s\lambda^4 [A_5 + sA_6 + s^2B_7] \\ - s^2\lambda^2 [A_4C_e^2 + sB_5 + s^2B_6] + s^4 [A_4 + sP_rS_c^2] = 0 \end{aligned} \quad (2.4.2)$$

Equation (2.4.2) is a quartic equation for λ^2 which can be solved explicitly. The complicated expressions, however, make the inversion difficult. It will be more expedient to obtain asymptotic expansions for the roots of the characteristic equation. The four positive roots have the following expansions for small s (which are appropriate for large-time inversions):

$$\begin{aligned} \lambda_1 &\sim \sqrt{s}\Lambda_1 [1 + 0(s)] \\ \lambda_2 &\sim \sqrt{s}\Lambda_2 [1 + 0(s)] \\ \lambda_3 &\sim \frac{s}{C_e} \left[1 - \frac{s}{4b_e^2} + 0(s^2) \right] \\ \lambda_4 &\sim \zeta_w + \frac{s}{C_w} \left[1 - \frac{s}{4b_w^2} + 0(s^2) \right] \end{aligned} \quad (2.4.3)$$

where

$$\Lambda_{1,2} \equiv \left[\frac{A_5 \pm \sqrt{A_5^2 - 4C_6 A_4 C_e^2}}{2C_6} \right]^{1/2} \quad (2.4.4)$$

$$\zeta_w \equiv \left[\frac{C_6}{1 - \delta^2} \right]^{1/2} \quad (2.4.5)$$

$$C_w \equiv \frac{2[C_6(1 - \delta^2)]^{3/2}}{C_6 A_7 (1 - \delta^2) - C_6^2 A_9 - A_5 (1 - \delta^2)^2} \quad (2.4.6)$$

$$\theta_1 \equiv \frac{A_7}{1 - \delta^2} + \frac{A_9 C_6}{(1 - \delta^2)} - \frac{A_5}{C_6}$$

$$\theta_2 \equiv \frac{A_8}{1 - \delta^2} - \frac{A_7 A_9}{(1 - \delta^2)^2} + \frac{A_5 A_7}{C_6^2} + \frac{A_9^2 C_6}{(1 - \delta^2)^3} - \frac{A_5^2 B_8}{C_6^3} \quad (2.4.7)$$

$$- \frac{A_6}{C_6} + \frac{A_4 (1 - \delta^2) C_e^2}{C_6^2}$$

$$b_e = \frac{C_e}{\sqrt{2}} \left[\frac{B_5}{A_4} - \frac{A_5}{A_4} \frac{1}{C_e^2} - \frac{P_r S^2 C_e^2}{A_4} \right]^{-1/2}$$

(2.4.8)

$$b_w = \left[\theta_1 \zeta_w^2 / (\theta_1^2 - 4 \zeta_w^2 \theta_2) \right]^{1/2}$$

The functions λ_1 and λ_2 vary to lowest order like \sqrt{s} and hence lead to purely diffusive behavior, such as might be associated with a temperature or mass fraction discontinuity. When Fick's Law holds, that is, when $\delta = K_X = K_F = 0$, the expressions for Λ_1 and Λ_2 simplify to

$$\Lambda_1 = \left[\frac{P_r S_c \{E_1 - (\beta_T - \beta\rho)(E_3 - Q)\}}{S_c E_1 + (\beta_T - \beta\rho)(P_r Q - S_c E_3)} \right]^{1/2} \quad (2.4.9)$$

$$\Lambda_2 = \sqrt{S_c} \quad (2.4.10)$$

The coefficients Λ_1 and Λ_2 essentially represent thermal and mass diffusivities. The thermal diffusivity limit $\Lambda_1 = \sqrt{P_r}$ is recovered by setting $Q = 0$, but the general form (2.4.9) shows the general effects of equilibrium chemical reactions plus a coupling with mass diffusivity through the appearance of S_c .

The function λ_3 varies like s to lowest order and hence leads to wave behavior. The wave speed is given by C_e which is thus identified as the equilibrium speed of sound. The diffusive spreading of the wave front is represented by the factor b_e in the second-order term of λ_3 .

The function λ_4 also leads to wave behavior, but this wave is damped by virtue of the lowest order term ζ_w . When Fick's Law of diffusion holds, the damping factor is given by

$$\zeta_w = \left[S_c E_1 + (\beta_T - \beta\rho)(P_r Q - S_c E_3) \right]^{1/2} \quad (2.4.11)$$

and is thus a function of thermal and mass diffusion through P_r and S_c , and the reaction rates through E_1 , β_T , and $\beta\rho$. The factor C_w represents the laminar flame speed, and the factor b_w represents the diffusive spreading. For Fick's Law, the flame speed C_w simplifies to

$$C_w = \frac{2 \zeta_w^3}{\zeta_w^2 \{S_c + \gamma \beta \rho (P_r Q - S_c E_3)\} + P_r (P_r - S_c) (\beta_T - \beta \rho) Q} \quad (2.4.12)$$

This laminar flame speed depends on thermal and mass diffusivities P_r and S_c and the reaction rates. Additional details of the equilibrium speed of sound and laminar flame speed shall be discussed in Sections 2.5 and 2.6.

2.5 Laminar Flame Propagation

Three mathematical formulations have been developed which attempt to predict the laminar flame structure and speed. The first method, introduced by Hirschfelder [31], aimed to solve the set of conservation equations for a stationary flame, with specified boundary conditions at the burned and unburned ends of the flame. It was shown that the propagation speed of a laminar flame corresponds to the eigenvalue of the governing boundary-value problem. The second method, proposed by Spalding [2], adopts a computing procedure to solve the equations of one-dimensional unsteady laminar flame propagation. Specifically, the method consists of setting up the time-dependent equations of conservation, assuming arbitrary initial profiles, and then solving the equations numerically. The iterative solution was continued until the profiles of the different dependent variables approached sufficiently close to a steady state. The asymp-

otics of large activation energy serves as the third method, but the notion was scarcely employed before the review article of Williams [6]. The method of matched asymptotic expansions [7,8] is used to obtain approximations for the rate of laminar flame propagation through a homogeneous, gaseous fuel mixture. The applications and flexibility of these methods have been proved, but they usually require fairly large number of restrictive assumptions. Consequently, there remains a need for a rational analysis of laminar flame theory in which diffusional effects, thermal effects, and transient behavior are all included. Linearized theory is intended for this purpose.

The formula for the dimensionless laminar flame speed in the present study has been established in (2.4.12). The dependence on the Damkohler's second number $\tau_{f_0}^*$ can be shown explicitly by manipulating (2.4.12), and we obtain

$$C_w = \frac{2 a_1^{3/2} \sqrt{\tau_{f_0}^*}}{(S_c a_1 + a_3) \tau_{f_0}^* + a_1 a_2} \quad (2.5.1)$$

where

$$a_1 \equiv S_c Y_{x_0}^x Y_{f_0}^f \left[\chi W_x \left(\frac{\chi}{Y_{x_0}} + \frac{g}{Y_{p_0}} \right) + f W_f \left(\frac{f}{Y_{f_0}} + \frac{g}{Y_{p_0}} \right) + \frac{\gamma Q^2}{(\gamma-1) \bar{W} L_e} + m E_3 \right] \quad (2.5.2)$$

$$a_2 \equiv \gamma Y_{x_0}^x Y_{f_0}^f m (P_r Q - S_c E_3) \quad (2.5.3)$$

$$a_3 \equiv P_r Q (P_r - S_c) Y_{x_0}^x Y_{f_0}^f \frac{\gamma Q}{(\gamma-1) \bar{W}} \quad (2.5.4)$$

and use has been made of equations (2.2.16), (2.2.17), and (2.2.18) among others. The Lewis number is defined by

$$L_e = S_c/P_r.$$

The wave associated with the wave speed C_w arises solely as a result of combustion processes. Within the framework of a linearized theory, this wave can be identified as a deflagration wave. Correspondingly, the wave associated with the equilibrium speed C_e is an embryonic detonation wave. Whereas the equilibrium speed is a well-known result and can be obtained from simpler considerations (see section 2.6), the concept of the deflagration wave as outlined here is a new approach. It is obtained from an entirely rational analysis. For instance, it is not necessary to suppose the pressure is a constant across this wave front. The behavior of the pressure will be a result of the analysis. There is no "cold-boundary" difficulty to deal with.

When the characteristic reaction time, $\tau_{f_0}^*$, that is, the second Damkohler number, is large, the deflagration wave speed C_w behaves asymptotically as

$$C_w \sim \frac{2a_1^{3/2}}{S_c a_1 + a_3} \frac{1}{\sqrt{\tau_{f_0}^*}} \quad (2.5.5)$$

This result is precisely true when $a_2 = 0$, or in particular when $m = 0$, where $m \equiv g - \chi - f$ is the net change of mole number during the chemical reaction. This functional dependency on $\tau_{f_0}^*$ is in agreement with conventional elementary

theories for obtaining laminar flame speeds, as might be anticipated from dimensional considerations [32].

When $\tau_{f_0}^*$ is sufficiently small, C_w deviates from the conventional behavior. This is illustrated in Fig. 2.1. The functional behavior of the flame speed with respect to $\tau_{f_0}^*$ depends on the value and algebraic sign of m in equation (2.5.3). As seen from Fig. 2.1, the curves for $m > 0$, $m < 0$, and $m = 0$ are distinctively different when $\tau_{f_0}^* < 10$. When $\tau_{f_0}^* > 10$, however, the behavior is the same for all values of m . It is possible that this behavior can account for some of the discrepancies between various theoretical models within themselves and also in comparison with experiment. Without detailed knowledge of the chemical kinetics, various theoretical results might differ by as much as 100% between themselves and with experiments [2]. As Clarke [13] has pointed out in connection with his detailed analyses of flame speeds for large activation energies, the coefficient of $(\tau_{f_0}^*)^{-1/2}$ in equation (2.5.5) is a complicated affair and depends in no very obvious manner on heat of combustion, species concentrations, Lewis number, and so forth. Equation (2.5.5) which is a special case of equation (2.5.1) valid for large $\tau_{f_0}^*$ (or $m = 0$), is certainly in agreement with this observation. The more general equation (2.5.1) is valid also when $\tau_{f_0}^*$ is not large and hence is not restricted to large activation energies.

In principle, equation (2.5.1) should provide numerical estimate for the laminar flame speed C_w . However,

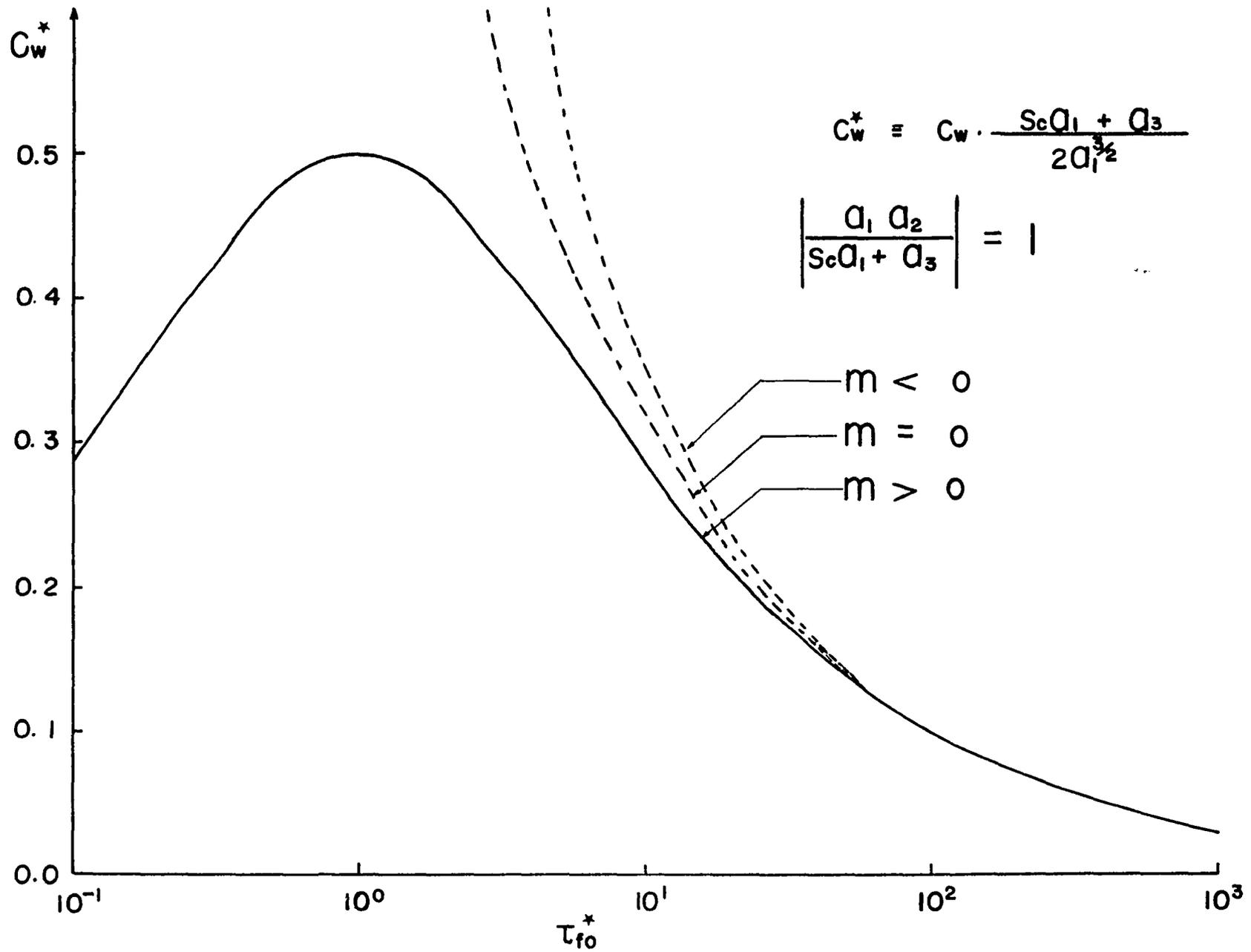


Figure 2.1 Variation of Non-dimensional Laminar Flame Speed with Second Damkohler Similarity Group

in practice, values of $\tau_{f_0}^*$ are so uncertain that equation (2.5.1) is more useful for estimating $\tau_{f_0}^*$ from experimental values of C_w . For example, let us consider an exothermically reacting mixture in an isolated system. If the mixture at a specified temperature and pressure is allowed to approach chemical equilibrium by a constant pressure process adiabatically, then the final temperature attained by the system is the adiabatic flame temperature T_f . Clearly T_f depends on the pressure, the initial temperature, and composition of the reactants. The final equilibrium mixture is employed as the initial mixture in the present linearized formulation. For specific chemical reaction, the equilibrium composition and the adiabatic flame temperature could be evaluated by an iterative procedure. The coefficients, a_1 , a_2 , and a_3 are then determined and the forward chemical reaction time τ_f could be estimated by measuring the speed C_w . Accordingly, the present linearized theory provides a new approach to study the influence of pressure, temperature, and composition on the flame speed, without the necessity of supposing the pressure is constant across the flame, and there is no "cold-boundary" difficulty to deal with. At this stage, it is seen that the present linearized approach is different from the conventional approach. In the conventional approach, the combustible mixture (at given temperature and pressure) contains fuel and oxidant only and there is no product initially. Either fuel or oxidant is consumed entirely after burning.

These are idealizations appropriate for large activation energies. Further, they give rise to the cold wall difficulty because the reaction rate never falls to zero if it follows the Arrhenius law. Essentially the situation in which combustion is not completed might prevail, and the mixture is really in an equilibrium state and at high temperature. Thus the initial conditions in the present problem may correspond to the final state of conventional combustion. Our problem might be viewed as an "after" combustion caused by a pressure or temperature disturbance imposed on a hot pre-burned equilibrium mixture.

It is interesting to note from formula (2.5.1) that, with $\tau_{f_0}^*$ roughly estimated between 10^2 to 10^4 (chemical forward reaction time lies in 10^{-6} to 10^{-8} sec, and the characteristic diffusion time is about 10^{-10} sec), C_w will then be in the range of 10^{-1} to 10^{-2} (flame speed is between 10^3 and 10^4 cm/sec). If C_w corresponds to about 10 cm/sec, then τ_f has about the value 10^{-2} sec. These results are larger than empirically determined flame speeds, which are in the range of tens to thousands cm/sec. Generally, however, these experimental results were not obtained from transient weak disturbance problems such as envisaged here.

2.6 Equilibrium Speed of Sound

The dimensionless equilibrium speed of sound, C_e , derived in the preceding section, can be obtained from simpler thermodynamic considerations. Following the work of Vincenti

and Kruger [26] for a dissociating gas, the Gibbs relation for our ternary reacting mixture is written as

$$Tds = dh - \frac{1}{\rho} dp - \left[(\mu_X - \mu_P) dY_X + (\mu_F - \mu_P) dY_F \right] \quad (2.6.1)$$

The quantity μ_α is called the chemical potential for species α . By means of the caloric equation of state in the functional form $h = h(p, \rho, Y_X, Y_F)$, we write the differential form

$$dh = \frac{\partial h}{\partial p} dp + \frac{\partial h}{\partial \rho} d\rho + \frac{\partial h}{\partial Y_X} dY_X + \frac{\partial h}{\partial Y_F} dY_F \quad (2.6.2)$$

equation (2.6.1) can also be written

$$Tds = \frac{\partial h}{\partial P} - \frac{1}{\rho} dP + \frac{\partial h}{\partial \rho} d\rho + \left[\frac{\partial h}{\partial Y_X} - (\mu_X - \mu_P) \right] dY_X + \left[\frac{\partial h}{\partial Y_F} - (\mu_F - \mu_P) \right] dY_F \quad (2.6.3)$$

For a reacting mixture in equilibrium, we have $Y_\alpha = Y_\alpha^*(P, \rho)$ and $(\mu_X - \mu_P) dY_X + (\mu_F - \mu_P) dY_F = 0$. It follows that the equilibrium speed of sound is determined by

$$a_{e0}^2 = \left[\left(\frac{\partial P}{\partial \rho} \right)_{s, Y_\alpha = Y_\alpha^*} \right]_0 = - \frac{P_0 \left[\frac{\partial h}{\partial \rho} + \frac{\partial h}{\partial Y_X} \frac{\partial Y_X^*}{\partial \rho} + \frac{\partial h}{\partial Y_F} \frac{\partial Y_F^*}{\partial \rho} \right]}{\rho_0 \left[\frac{\partial h}{\partial P} + \frac{\partial h}{\partial Y_X} \frac{\partial Y_X^*}{\partial P} + \frac{\partial h}{\partial Y_F} \frac{\partial Y_F^*}{\partial P} - \frac{P_0}{\rho_0} \right]} \quad (2.6.4)$$

where the derivatives $\frac{\partial h}{\partial \rho}$, $\frac{\partial h}{\partial P}$, $\frac{\partial h}{\partial Y_\alpha}$ are evaluated at the ambient equilibrium state and P, ρ have been normalized.

The calculation of a_e for the specific ternary system in this study can be established by evaluating the

derivatives in equation (2.6.4). First, from the caloric equation of state (2.1.15), we have the differential form

$$\begin{aligned} dh = & \left[(h_X - h_P) - C_{pO}^T \alpha_X \right] dY_X + \left[(h_F - h_P) - C_{pO}^T \alpha_F \right] dY_F \\ & + C_{pO}^T dP - C_{pO}^T d\rho \end{aligned} \quad (2.6.4)$$

where use has been made of the linearized thermal equation of state (2.2.11) to eliminate T. This gives

$$\frac{\partial h}{\partial Y_X} = (h_X - h_P) - C_{pO}^T \alpha_X, \quad \frac{\partial h}{\partial P} = C_{pO}^T \quad (2.6.5)$$

$$\frac{\partial h}{\partial Y_F} = (h_F - h_P) - C_{pO}^T \alpha_F, \quad \frac{\partial h}{\partial \rho} = -C_{pO}^T$$

The explicit form of function $Y_\alpha^*(P, \rho)$ is found from the fact that linearized rate of reaction function \tilde{R} is equal to zero under equilibrium condition and the changes of species fraction are related by $Y_X/Y_F = \chi W_{X\zeta} / f W_{F\zeta}$ where ζ is the degree of advancement. The result is given by

$$\begin{aligned} Y_X^* &= \frac{\chi W_X}{E_1} \left[(\beta_\rho - \beta_T) \rho + \beta_T P \right] \\ Y_F^* &= \frac{f W_F}{E_1} \left[(\beta_\rho - \beta_T) \rho + \beta_T P \right] \end{aligned} \quad (2.6.6)$$

hence it follows that

$$\begin{aligned} \frac{\partial Y_X^*}{\partial \rho} &= \frac{\chi W_X}{E_1} (\beta_\rho - \beta_T), \quad \frac{\partial Y_X^*}{\partial P} = \frac{\chi W_X}{E_1} \beta_T \\ \frac{\partial Y_F^*}{\partial \rho} &= \frac{f W_F}{E_1} (\beta_\rho - \beta_T), \quad \frac{\partial Y_F^*}{\partial P} = \frac{f W_F}{E_1} \beta_T \end{aligned} \quad (2.6.7)$$

Substituting these derivatives into (2.6.4), and after some simple algebraic manipulation, we find the dimensional equilibrium speed of sound:

$$a_{e_0}^2 = \frac{\gamma P_0}{\rho_0} \frac{E_1 + (\beta_T - \beta_\rho)(Q - E_3)}{E_1 + \gamma \beta_T(Q - E_3)} \quad (2.6.8)$$

This final result is exactly the same (after normalization by the frozen speed of sound) as that in the governing equation (2.3.18). Note that the equilibrium speed C_e is independent of τ_f^* .

CHAPTER III

APPLICATION TO HOT-SURFACE IGNITION OF GASES

3.1 Statement of the Problem

When a gas mixture capable of an exothermic reaction is heated locally and rapidly under various modes of energy supply, such as an electrical spark, a hot vessel wall, a pocket of hot gas, or a pilot flame, a flame front can be initiated in the vicinity of the energy source and propagated into the rest of the mixture. A considerable amount of study has been given to problems which pertain to the ignition of reacting condensed substances [33,34]. Relatively few studies have dealt with the problem of ignition of gases which is more complicated than that for condensed-phase ignition, because the convective motions in gases must be taken into account. In most problems of ignition of gases studies in the past [35,36,37], attention has been directed primarily to the laws of ignition, namely, the critical conditions for the establishment of steady-state flame in a gas mixture and the quenching and ignition limits.

Shkadinskii and Barzykin [35] have considered the problem of hot-surface ignition of gases with allowance for

diffusion and hydrodynamics by means of numerical work. The treatment is confined to the assumption of constant pressure, it is valid after the pressure wave has left the reaction zone. In the present analysis, a similiar problem will be studied with a different viewpoint as mentioned in Section 2.5, and the emphasis will be on the problem of gasdynamic aspects of ignition which is becoming of importance in understanding combustion noise. The particular purpose of this chapter is to contribute to a qualitative picture of nonequilibrium dissipative phenomena involved in complicated ignition process, stressing asymptotic behaviors which display certain consequences of heating conditions at ignition source. The specific ignition problem described above may be simulated as follows. At the initial instant, a chemically reacting gas mixture that is in a state of chemical equilibrium and semi-infinite in extent is brought into contact with a hot surface whose temperature exceeds the initial temperature of the mixture; the subsequent response induced in the gas mixture is then to be determined. Two fundamentally different types of surface conditions are considered:

- (a) constant surface temperature; the heat flow at the surface falls with time,
- (b) constant heat flow through the surface, the surface temperature increases.

The initial conditions for the ignition problem are that all perturbation variables are zero at $\tau = 0$. The boundary con-

ditions at the hot-surface, which we take to be non-catalytic and impermeable, are

$$T = F(\tau), u = 0, \text{ and } Y_{\alpha X} = 0 (\alpha = X, F) \text{ for } \tau > 0, x = 0 \quad (3.1.1)$$

Finally, all perturbations must vanish at infinity. The problem facing us is to solve the governing equation (2.3.18) subject to the above initial and boundary conditions.

3.2 Laplace-Transform Analysis

A solution can be obtained by taking the Laplace transform with respect to τ followed by solving of the ordinary differential equation in the space variable x . If $\bar{\phi}(x, s)$ denotes the Laplace transform with respect to time of $\phi(x, \tau)$, the transformed solution of (2.3.18) is

$$\bar{\phi}(x, s) = \sum_{n=1}^4 B_n \exp \left[-\lambda_n(s)x \right] \quad (3.2.1)$$

where $\lambda_1, \lambda_2, \lambda_3$ and λ_4 are the positive roots of the quartic equation (2.4.2) for λ^2 . Their asymptotic expansions in the limit of $s \rightarrow 0$ have been derived in (2.4.3)-(2.4.8), and $B_1, B_2, B_3,$ and B_4 are arbitrary constants of integration. The transformed solutions for pressure and density are found directly from equation (2.3.2) and (2.3.3):

$$\bar{P}(x, s) = \gamma \sum_{n=1}^4 (\lambda_n^2 - s) B_n \exp(-\lambda_n x) \quad (3.2.2)$$

$$\bar{\rho}(x, s) = -\frac{1}{s} \sum_{n=1}^4 \lambda_n^2 B_n \exp(-\lambda_n x) \quad (3.2.3)$$

The particular integrals of the transforms of simultaneous equations (2.2.7) and (2.2.8) are obtained in the form

$$\begin{aligned}\bar{Y}_X &= \sum_{n=1}^4 \Pi_{nX} B_n \exp(-\lambda_n x) \\ \bar{Y}_F &= \sum_{n=1}^4 \Pi_{nF} B_n \exp(-\lambda_n x)\end{aligned}\tag{3.2.4}$$

where

$$\begin{aligned}\Pi_{nX} &= -S_C \gamma \beta_T (\chi W_X - \delta f W_F) \frac{\lambda_n^2 (\lambda_n^2 - s)}{\Lambda_n} + \frac{S_C}{s} (\beta \rho - \beta_T) (\chi W_X - f W_F) \frac{\lambda_n^4}{\Lambda_n} \\ &+ S_C^2 \gamma \beta_T (\chi W_X s) \frac{\lambda_n^2 - s}{\Lambda_n} - S_C^2 (\beta \rho - \beta_T) \chi W_X \frac{\lambda_n^2}{\Lambda_n} \\ \Pi_{nF} &= -S_C \gamma \beta_T (f W_F - \delta \chi W_X) \frac{\lambda_n^2 (\lambda_n^2 - s)}{\Lambda_n} + \frac{S_C}{s} (\beta \rho - \beta_T) (f W_F - \delta \chi W_X) \frac{\lambda_n^4}{\Lambda_n} \\ &+ S_C^2 \gamma \beta_T (f W_F s) \frac{\lambda_n^2 - s}{\Lambda_n} - S_C^2 (\beta \rho - \beta_T) f W_F \frac{\lambda_n^2}{\Lambda_n} \\ \Lambda_n &= (1 - \delta^2) \lambda_n^4 - S_C (2s + E_1 - \delta E_2) \lambda_n^2 + S_C^2 (s^2 + s E_1)\end{aligned}$$

(3.2.5)

and pressure diffusion has been ignored. The transform of the temperature is then determined by means of equation (2.2.11). The transform of the velocity is determined by $\bar{u} = \bar{\phi}'_x$.

The four constants $B_1, B_2, B_3,$ and B_4 in the above transformed expressions are determined by imposing the trans-

formed boundary conditions (3.1.1) at the hot-surface. These conditions provide four equations for the four unknowns:

$$\begin{aligned} \sum_{n=1}^4 \left[\gamma (\lambda_n^2 - s) + \frac{\lambda_n^2}{s} - \alpha_X \Pi_{nX} - \alpha_F \Pi_{nF} \right] B_n &= f(s) \\ \sum_{n=1}^4 \lambda_n B_n &= 0 \\ \sum_{n=1}^4 \lambda_n \Pi_{nX} B_n &= 0 \\ \sum_{n=1}^4 \lambda_n \Pi_{nF} B_n &= 0. \end{aligned} \tag{3.2.6}$$

Solving these equations yields

$$\begin{aligned} B_1 &= \frac{f(s) \lambda_2 \lambda_3 \lambda_4}{\Delta} (\Pi_{3X} \Pi_{4F} + \Pi_{2X} \Pi_{3F} + \Pi_{4X} \Pi_{2F} - \Pi_{3X} \Pi_{2F} - \Pi_{2X} \Pi_{4F} - \Pi_{4X} \Pi_{3F}) \\ B_2 &= \frac{-f(s) \lambda_3 \lambda_4 \lambda_1}{\Delta} (\Pi_{4X} \Pi_{1F} + \Pi_{3X} \Pi_{4F} + \Pi_{1X} \Pi_{3F} - \Pi_{4X} \Pi_{3F} - \Pi_{3X} \Pi_{1F} - \Pi_{1X} \Pi_{4F}) \\ B_3 &= \frac{f(s) \lambda_4 \lambda_1 \lambda_2}{\Delta} (\Pi_{1X} \Pi_{2F} + \Pi_{4X} \Pi_{1F} + \Pi_{2X} \Pi_{4F} - \Pi_{1X} \Pi_{4F} - \Pi_{4X} \Pi_{2F} - \Pi_{2X} \Pi_{1F}) \\ B_4 &= \frac{-f(s) \lambda_1 \lambda_2 \lambda_3}{\Delta} (\Pi_{2X} \Pi_{3F} + \Pi_{1X} \Pi_{2F} + \Pi_{3X} \Pi_{1F} - \Pi_{2X} \Pi_{1F} - \Pi_{1X} \Pi_{3F} - \Pi_{3X} \Pi_{2F}) \end{aligned} \tag{3.2.7}$$

where

$$\Delta \equiv \begin{vmatrix} \psi_1 & \psi_2 & \psi_3 & \psi_4 \\ \lambda_1 & \lambda_2 & \lambda_3 & \lambda_4 \\ \lambda_1 \Pi_{1X} & \lambda_2 \Pi_{2X} & \lambda_3 \Pi_{3X} & \lambda_4 \Pi_{4X} \\ \lambda_1 \Pi_{1F} & \lambda_2 \Pi_{2F} & \lambda_3 \Pi_{3F} & \lambda_4 \Pi_{4F} \end{vmatrix} \tag{3.2.8}$$

and

$$\psi_n = \gamma(\lambda_n^2 - s) + \frac{\lambda_n^2}{s} - \alpha_X \Pi_{nX} - \alpha_F \Pi_{nF} \quad (3.2.9)$$

The solution for the transformed problem is now complete. The complicated form of the transformed solution we encounter makes the exact inversion impossible. However, asymptotic approximations valid for large values of the time can be developed by expanding all transforms for small s [38]. In the limit $s \rightarrow 0$, the roots of the characteristic equation have the expansions given in (2.4.3) and the corresponding expansions for B_1, B_3, B_4 are (for $\delta=0$).

$$\begin{aligned} B_1 &\sim f(s) \frac{h}{\Lambda_1^2} \left[1 + E_0 s^{1/2} + E_0^* s^{1/2} + o(s) \right] \\ B_3 &\sim -f(s) \frac{C_e h}{\Lambda_1} s^{-1/2} + o(s^{1/2}) \\ B_4 &\sim -f(s) \frac{E_0^* (P_r Q - S_c E_3)}{P_r Q \zeta_w^2} + s^{3/2} + o(s^{5/2}) \end{aligned} \quad (3.2.10)$$

where

$$\begin{aligned} h &= \frac{E_1}{E_1 - (\beta_T - \beta_\rho) E_3} \\ E_0 &= \frac{E_1 C_e [E_1 - \gamma E_1 + \gamma \beta_\rho (Q - E_3) - E_3 (\beta_T - \beta_\rho - \gamma \beta_T)] [S_c E_1 + (\beta_T - \beta_\rho) (P_r Q - S_c E_3)]^{1/2}}{[E_1 - (\beta_T - \beta_\rho) E_3] [E_1 + (\beta_T - \beta_\rho) (Q - E_3)]^{3/2} (P_r S_c)^{1/2}} \\ E_0^* &= \frac{P_r^{3/2} Q (\beta_\rho - \beta_T) [E_1 + (\beta_T - \beta_\rho) (Q - E_3)]^{1/2}}{S_c^{1/2} [E_1 - (\beta_T - \beta_\rho) E_3] [S_c E_1 + (\beta_T - \beta_\rho) (P_r Q - S_c E_3)]} \end{aligned} \quad (3.2.11)$$

and it is found that B_2 vanishes identically when $\delta=0$ (see

Appendix A). The transformed field variables after having been expanded for small s have the lowest-order terms represented in the following form:

$$\bar{T}(x,s) \sim f(s) \left[\exp(-\lambda_1 x) + E_0 s^{1/2} \{ \exp(-\lambda_1 x) - \exp(-\lambda_3 x) \} + E_0^* s^{1/2} \{ \exp(-\lambda_1 x) - \exp(-\lambda_4 x) \} \right] \quad (3.2.12)$$

$$\bar{P}(x,s) \sim \frac{f(s)\gamma h}{\Lambda_1^2} \left[(\Lambda_1^2 - 1) s \exp(-\gamma_1 x) + C_e \Lambda_1 s^{1/2} \exp(-\lambda_3 x) + \frac{(\beta_T - \beta_\rho)(P_r Q - S_c E_3) \Lambda_1^3}{S_c E_1 \zeta_w} s^{3/2} \exp(-\lambda_4 x) \right] \quad (3.2.13)$$

$$\bar{u}(x,s) \sim f(s) s \frac{h}{\Lambda_1} \left[\exp(-\lambda_3 x) - \exp(-\lambda_1 x) \right] \quad (3.2.14)$$

$$\frac{\bar{Y}_X(x,s)}{W_X} \sim f(s) \frac{(\beta_T - \beta_\rho) h}{E_1} \left[\exp(-\lambda_1 x) - \frac{\Lambda_1}{\zeta_w} s^{1/2} \exp(-\lambda_4 x) \right] \quad (3.2.15)$$

3.3 Ignition at a Constant Surface Temperature

We first consider the case in which the wall temperature does not change with time. The condition may be described by $f(s) = \Delta_T/s$, where Δ_T is the dimensionless temperature of the source. The transformed problem can now be inverted by means of standard Laplace-transform tables and by the approximation method proposed by Rasmussen [22]. With the use of expressions (3.2.12)-(3.2.15), the general formulas for the asymptotic behavior of the large-time solution are found to be

$$\begin{aligned} \frac{T(x,\tau)}{\Delta_T} \sim \operatorname{erfc}\left(\frac{\Lambda_1 x}{\sqrt{4\tau}}\right) + E_0 \left[\frac{\exp\left[-\frac{\Lambda_1^2 x^2}{4\tau}\right]}{\sqrt{4\tau}} - I(x,\tau;b_e,C_e) \right] \\ + E_0^* \left[\frac{\exp\left[-\frac{\Lambda_1^2 x^2}{4\tau}\right]}{\sqrt{\pi\tau}} - \exp(-\zeta_w x) I(x,\tau;b_w,C_w) \right] \\ + o(\tau^{-3/2}) \end{aligned} \quad (3.3.1)$$

$$\frac{P(x,\tau)}{\Delta_T} \sim \frac{\gamma h C_e}{\Lambda_1} I(x,\tau;b_e,C_e) + o(\tau^{-3/2}) \quad (3.3.2)$$

$$\begin{aligned} \frac{u(x,\tau)}{\Delta_T} \sim \frac{h}{\Lambda_1} \left[I(x,\tau;b_e,C_e) - \frac{\exp\left[-\frac{\Lambda_1^2 x^2}{4\tau}\right]}{\sqrt{\pi\tau}} \right] \\ + o(\tau^{-3/2}) \end{aligned} \quad (3.3.3)$$

$$\begin{aligned} \frac{Y_X(x,\tau)}{\chi W_X \Delta_T} \sim \frac{(\beta_T - \beta_\rho) h}{E_1} \left[\operatorname{erfc}\left(\frac{\Lambda_1 x}{\sqrt{4\tau}}\right) - \frac{\Lambda_1}{\zeta_w} \exp(-\zeta_w x) I(x,\tau;b_w,C_w) \right] \\ + o(\tau^{-3/2}) \end{aligned} \quad (3.3.4)$$

where

$$I(x,\tau;b,C) \equiv \frac{bx}{\pi C} \int_0^\tau \frac{e^{-b^2(t-x/c)^2/t} dt}{\sqrt{\tau-t} t^{3/2}} \quad (3.3.5)$$

Several interesting features of wave propagation may be noted from the quadrature (3.3.5) that appears in the above asymptotic formulas. The quadrature was evaluated numerically. The function $\sqrt{\pi\tau} * I(x,\tau;b,C)$ is shown in Fig. 3.1 as a function of x/τ for various instants of time. Before we enter into a discussion of the details of the behavior of

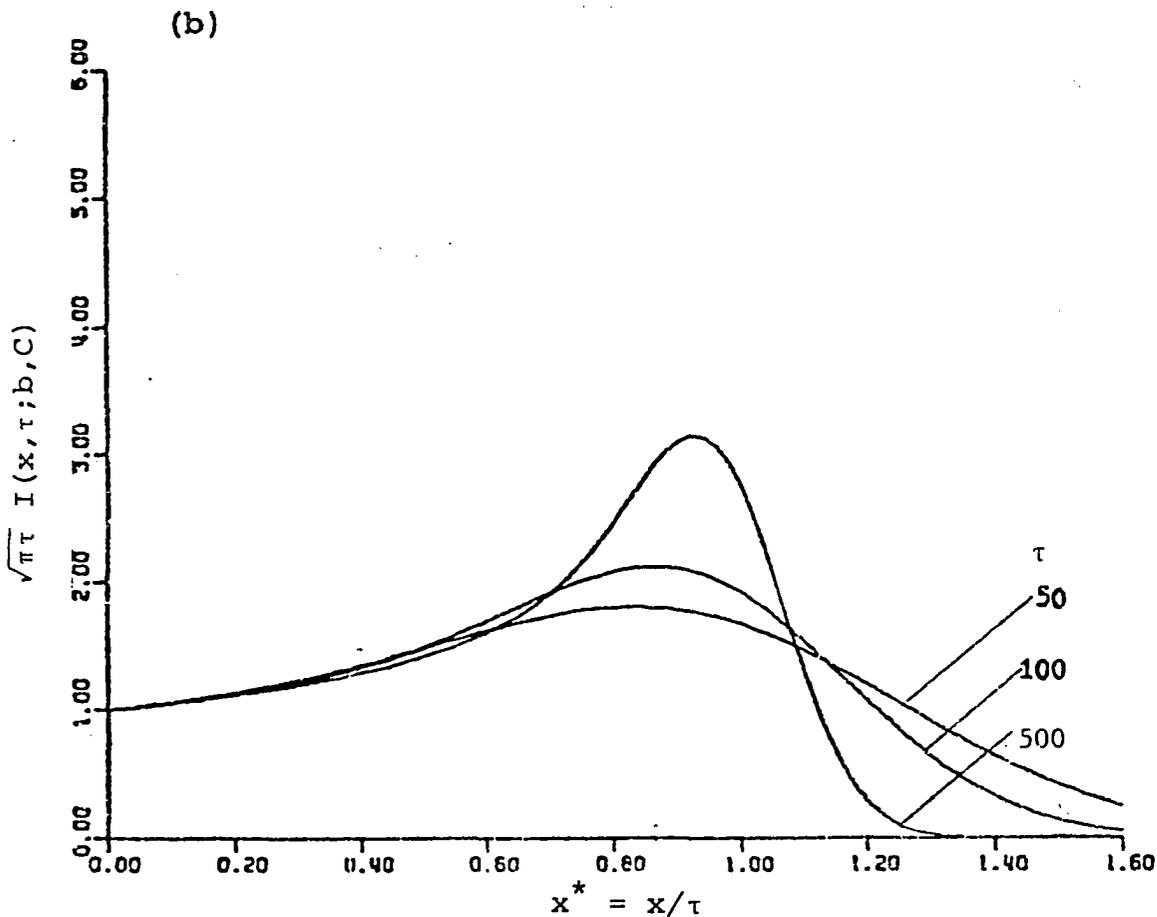
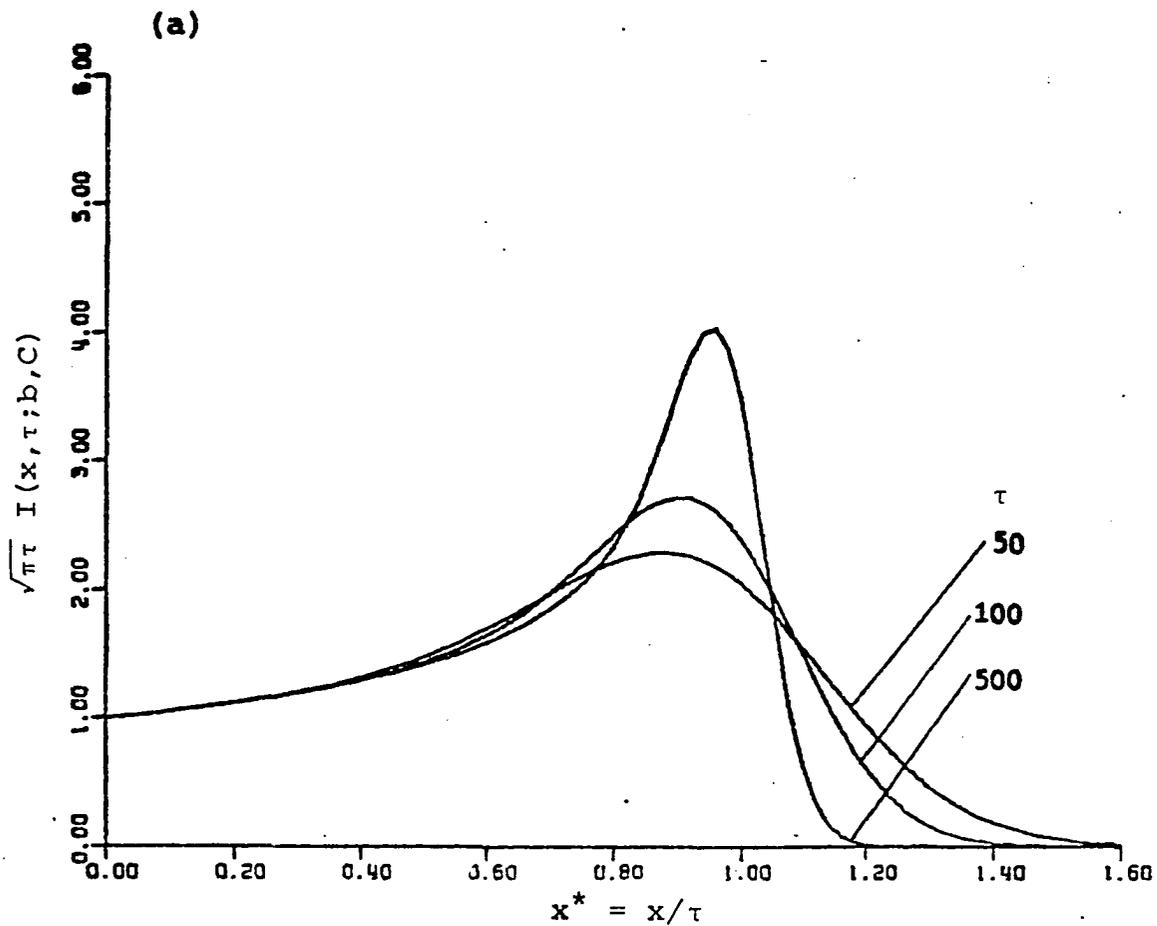


Figure 3.1 Diffusive Wave Behavior of Function $I(x, \tau; b, C)$:
(a) $b=0.5, C=1.0$ (b) $b=0.3, C=1.0$

the wave function $I(x, \tau; b, C)$, it is helpful to examine its asymptotic behavior in different domains. The integral (3.3.5) is evaluated asymptotically for three limiting cases: $x/C_\tau < 1$, $x/C_\tau \sim 1$, and $x/C_\tau > 1$, by the Laplace's method [47].

It is found that

$$I(x, \tau; b, C) \sim \frac{1}{2\sqrt{\pi\tau}} \frac{1}{\sqrt{1-x/C_\tau}} \operatorname{erfc} \left\{ -\sqrt{\frac{4b^2 x^2}{C_\tau^2} \left(1 - \frac{x}{C_\tau}\right)} \right\} \quad (3.3.6)$$

(for $x/C_\tau < 1$ and not too close to 1)

$$I(x, \tau; b, C) \sim \frac{\sqrt{b}}{2\pi} \frac{e^{-b^2 \tau (x/C_\tau - 1)^2}}{\tau^{1/4}} \frac{\Gamma(\frac{1}{4})}{1 + b\sqrt{\tau} (x/C_\tau - 1) \Gamma(\frac{3}{4}) / \Gamma(\frac{1}{4})} \quad (3.3.7)$$

(for $x/C_\tau \sim 1$)

$$I(x, \tau; b, C) \sim \frac{1}{\sqrt{\pi\tau}} \frac{x}{C_\tau} \frac{e^{-b^2 \tau (x/C_\tau - 1)^2}}{\sqrt{x^2/C_\tau^2 - 1}} \quad (3.3.8)$$

(for $x/C_\tau > 1$ and not too close to 1)

The magnitude of the wave function is largest near the wave front ($x/\tau = C$). The magnitude is associated with the strength of the generating disturbance. Since the generating disturbance decreases with time, the strongest part of the disturbance is at the wave front, which was generated earliest. The wave front is diffused out because of dissipation, and the diffusive spreading is reflected through the factor b . For a fixed value of x/τ , $I(x, \tau; b, C)$ dies out approximately like $\tau^{-1/2}$ when $x/C_\tau < 1$ (not too close to 1), like $\tau^{-1/4}$ near the wave front ($x/C_\tau \sim 1$), and decays exponentially when $x/C_\tau > 1$

(not too close to 1). These have been shown from the expressions (3.3.6)-(3.3.8).

The resulting process associated with hot-surface ignition of gases in most real cases may be described as follows. The temperature jump at the boundary causes a pressure wave that moves with the equilibrium speed of sound through the ambient gas. The heat flow from the hot-surface raises the adjacent layers of gas to a higher temperature and initiates an exothermic chemical reaction. Subsequently, the thermal energy released in the reaction zone accelerates the reaction, and a nonstationary combustion front is formed. Since the equilibrium speed of sound ($0[10^5 \text{ cm/sec}]$) is much higher than that of the laminar flame ($0[10^1 \sim 10^3 \text{ cm/sec}]$), the equilibrium wave leaves the heating and reaction zones and has no further effect on the process. Behind the wave, a gas velocity corresponding to the expansion of the heated gas and a pressure equal to the starting pressure are established.

For the purpose of illustration, the pertinent parameters appear in the asymptotic solutions will be chosen as:

$$E_o = 1.0, \quad E_o^* = 10.0, \quad \Lambda_1 = 0.915, \quad \zeta_w = 0.01$$

$$b_e = 0.6, \quad C_e = 0.95, \quad b_w = 0.5, \quad C_w = 0.20$$

The asymptotic solutions we have developed illustrate these thermal mechanisms qualitatively. The distribution of the

perturbation temperature is plotted in Figure 3.2 as a function of $x^* = x/\tau$ for various times and for selected values of the parameters. It should be noted that the coefficient E_0^* associated with the combustion front term is proportional to the effective heat of reaction, whereas E is not. The thermal boundary layer spreads from the hot-surface as the square root of time and is given by the first term in (3.3.1). This is the usual term obtained in the time-dependent problem of heat conduction when there is a temperature jump on the boundary surface, except the thermal diffusivity is modified by the effects of the chemical reaction and mass diffusion. The contribution from the pressure wave is given by $I(x, \tau; b_e, C_e)$ led by E_0 in equation (3.3.1). The term associated with $I(x, \tau; b_w, C_w)$ in equation (3.3.1) describes the contribution from the exothermic chemical reaction; its space-time distribution is similar to those previously examined by Averson et al. [39] and Shkadinskii and Barzykin [35]. It should be pointed out that only the reaction zone is represented in the work of these authors. In the real ignition cases, as the flame front moves away from the wall the heat flux into the burning zone decreases, but the heat released in the chemical reaction compensates for the heat transferred to the colder part of the gas and then raises the temperature to such a point that the reaction accelerates sharply and a nonstationary combustion front is formed. The temperature perturbation generated in the reaction zone in the present case is predominately due to

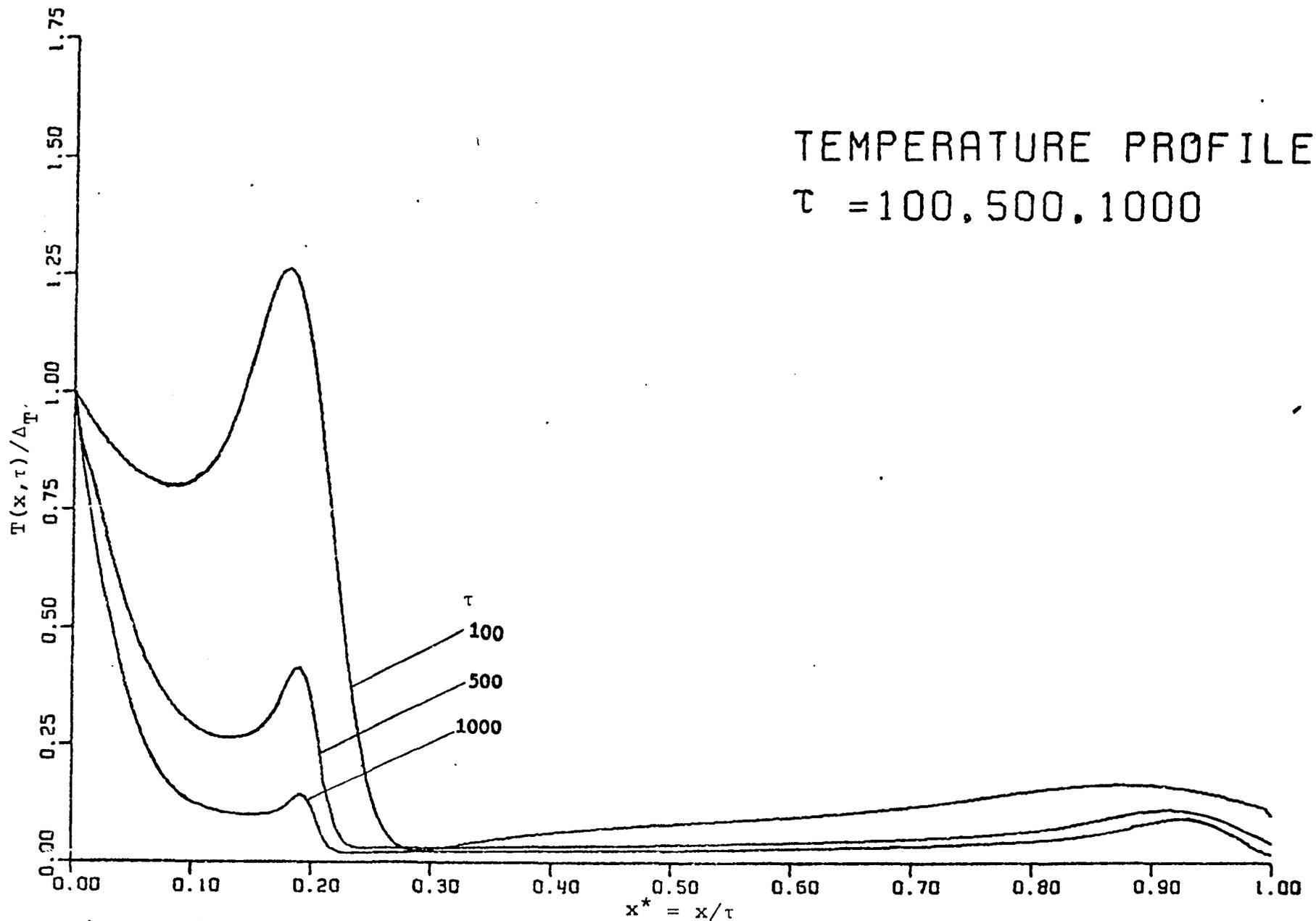


Figure 3.2 Long-time Behavior of the Temperature Perturbation for Ignition of Gases at a Constant Surface Temperature

the presence of thermal flux from the hot wall into the burning zone. The rate of the thermal flux decreases with time for the case of constant surface temperature, and the rate of chemical reaction and the heat released in the reaction zone decrease. Therefore, the amplitude of the temperature perturbation in the burning zone decreases with time. Furthermore, as the flame front moves away from the hot wall the heat flux into the burning zone decreases, and the induced chemical reaction and temperature perturbation also decrease. These results are described by the damping term contained in the chemical contribution such that the induced perturbation dies out exponentially with distance from the hot-surface. The lower-order diffusion terms, that is $\exp\left(-\frac{\Lambda_1^2 x^2}{4\tau}\right)/\sqrt{\pi\tau}$, appear in the equation (3.3.1) are the contributions of the thermal expansion of the gas, associated with the pressure wave and the chemical reaction. They cause a fall in temperature.

The function associated with the gasdynamic wave dominates the pressure distribution. The resulting pressure distribution is quite like that in Fig. 3.1. The pressure variation induced by the flame propagation is higher order and has been ignored in the asymptotic expression (3.3.2). Thus we may conclude that the conventional assumption of constant pressure through the flame is an acceptable approximation.

Fig. 3.3 gives the space-time distribution of the perturbation velocity for selected parameters. Physically, the hot surface transfers heat to the gas, causing a pressure wave and initiating an exothermic chemical reaction. The expansion of the gas, associated with the pressure wave and the chemical reaction, causes a motion away from the wall. However, the velocity caused by chemical conversion itself and the thermal expansion associated with the chemical reaction are higher order and has been disregarded in the asymptotic expression (3.3.3). Thus, the dominant contributions are from the gasdynamic mechanism and the resulting velocity distribution is similar to that of the inert system; there is a velocity peak near the pressure wave front and the velocity doesn't vary with distance in a region between the wave front and just outside the velocity boundary layer, as shown in Fig. 3.3. It should be noted that the induced velocity increases with increase in temperature jump ΔT , and the amplitude decreases with time for the same reasons as that for the temperature perturbation.

The space-time distribution of species concentration of oxidant is represented in Fig. 3.4. The mass-diffusion boundary layer spreads from the hot-surface through the combined effects of diffusion. The reaction zone is centered at $x = C_w \tau$ and spreads parabolically with time. A feature of the space-time distribution of species concentration of oxidant is its increase in time to the value of the initial equilibrium state.

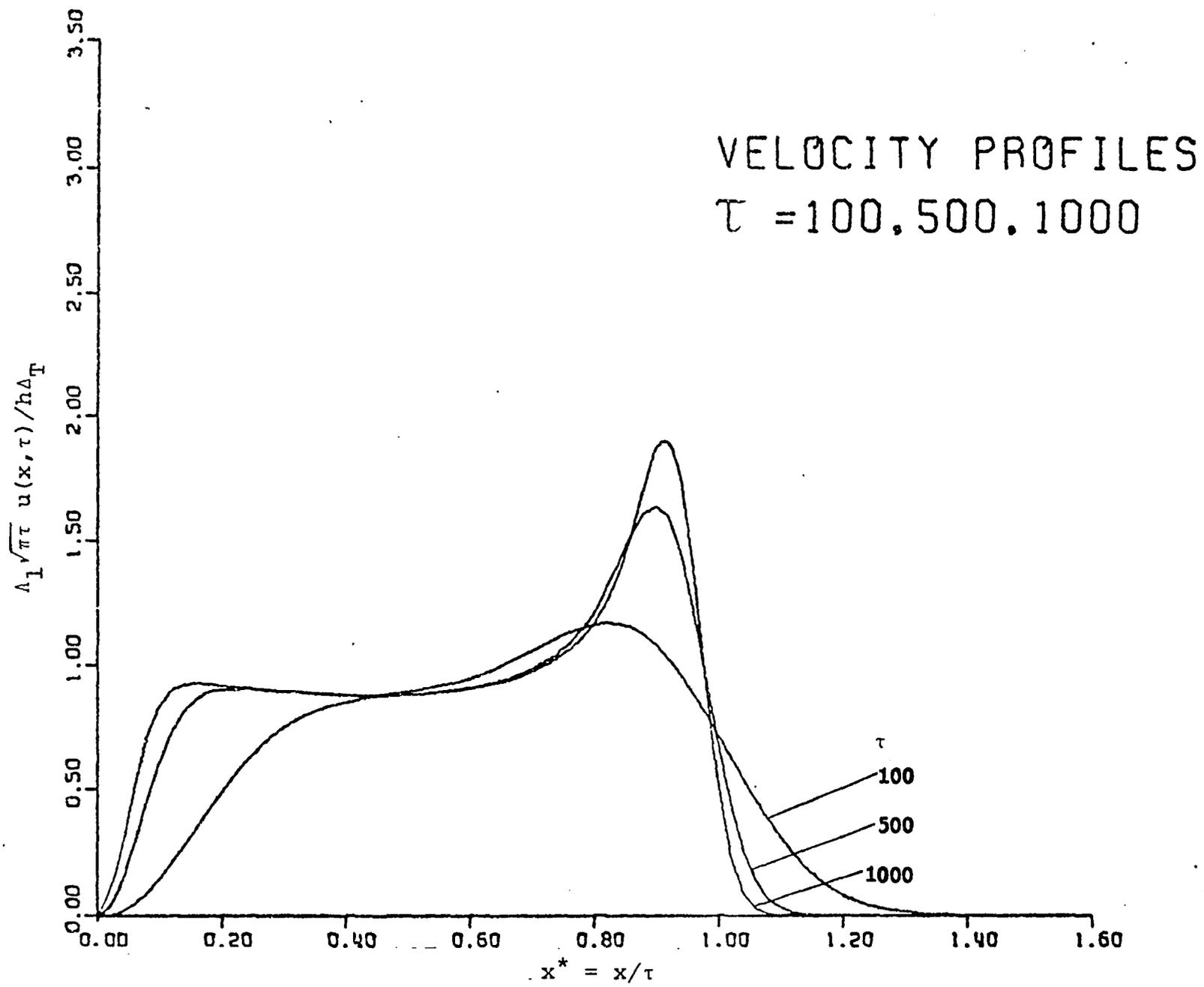


Figure 3.3 Long-time Behavior of the Velocity Perturbation for Ignition of Gases at a Constant Surface Temperature

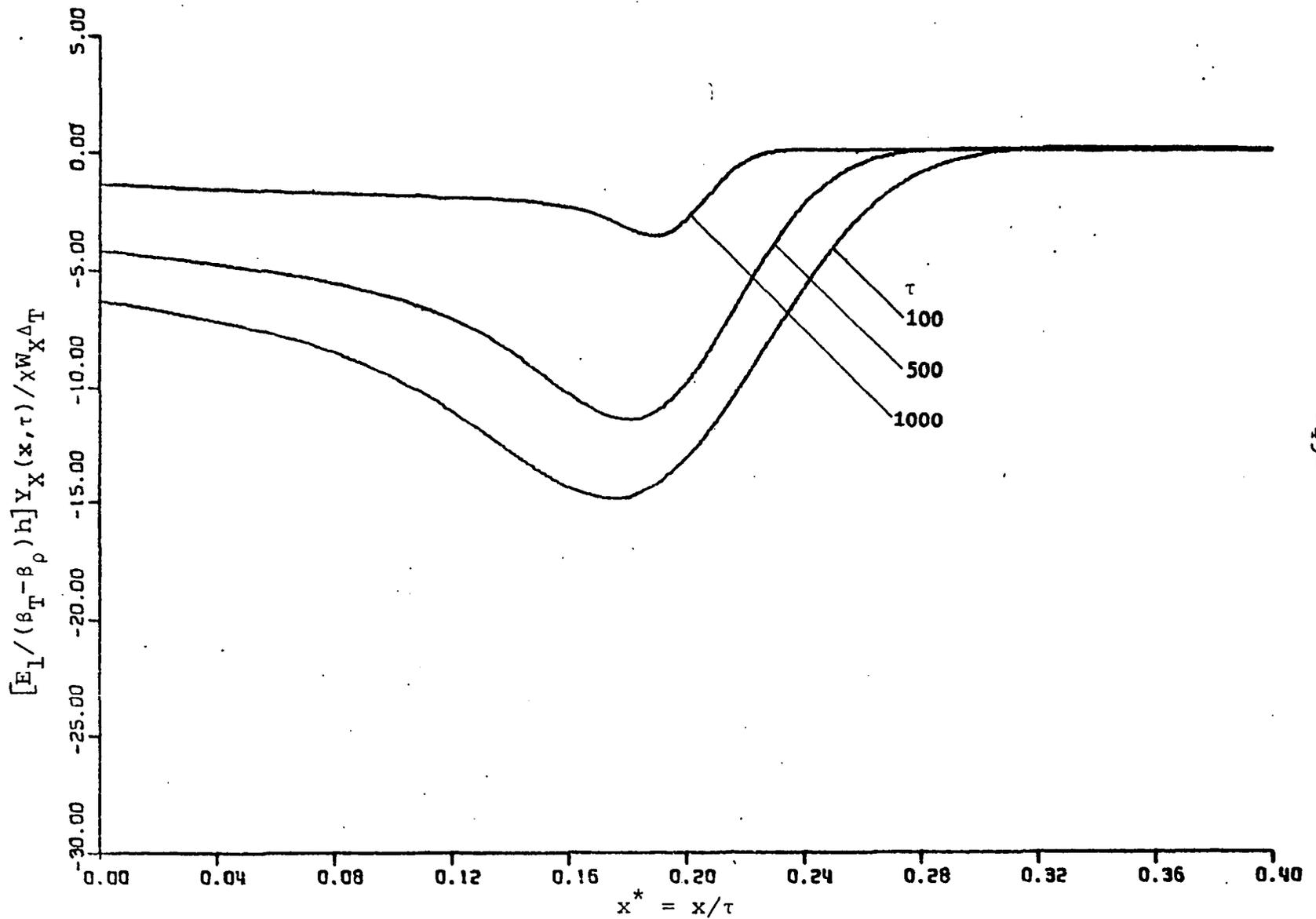


Figure 3.4 Long-time Behavior of Species Concentration of Oxidant for Ignition of Gases at a Constant Surface Temperature

This is because the flow of heat from the wall decreases with time; consequently, the induced chemical reaction is incapable of self-acceleration if the heat released due to the exothermic reaction is not enough. Practically, the present problem may correspond to situations in which the gaseous mixture cannot be ignited or, if ignited, is incapable of sustained burning. Such a correspondence might be important in various situations where "degenerate" combustion takes place.

There is a limiting case in which the chemical reaction does not occur, such as that of an inert mixture; the resulting flow field then reduces to the problem of thermally driven acoustic phenomena. The results for this case are expressed as

$$\frac{T(x, \tau)}{\Delta_T} \sim \operatorname{erfc} \left(\frac{\sqrt{P_r} x}{\sqrt{4\tau}} \right) + \frac{\gamma-1}{\sqrt{P_r}} \left[I(x, \tau; b, C_e=1) - \frac{\exp \left[-\frac{P_r x^2}{4\tau} \right]}{\sqrt{\pi\tau}} \right] \quad (3.3.9)$$

$$\frac{P(x, \tau)}{\Delta_T} \sim \frac{\gamma}{\sqrt{P_r}} I(x, \tau; b, C_e=1) \quad (3.3.10)$$

$$\frac{u(x, \tau)}{\Delta_T} \sim \frac{1}{\sqrt{P_r}} \left[I(x, \tau; b, C_e=1) - \frac{\exp \left[-\frac{P_r x^2}{4\tau} \right]}{\sqrt{\pi\tau}} \right] \quad (3.3.11)$$

where $b \equiv (2\gamma)^{-1/2}$. Thus the resulting field is composed of the diffusive wave propagation, thermal conduction, and thermal expansion.

3.4 Ignition by a Constant Heat Flow

In the case of constant heat flow through the surface, the surface temperature increases continually. The effect of constant heat flux may be characterized unambiguously by the result that the surface temperature is a particular function of time. It can be shown that the function is described by $F(\tau) = \frac{2}{\sqrt{\pi}} \sqrt{\tau}$ (for the sake of simplicity). To lowest order, the asymptotic approximations that satisfy the conditions on the hot-surface are then found to be

$$\begin{aligned} T(x, \tau) \sim & \sqrt{\frac{4\tau}{\pi}} \exp\left[-\frac{\Lambda_1^2 x^2}{4\tau}\right] - \Lambda_1 x \operatorname{erfc}\left(\frac{\Lambda_1 x}{\sqrt{4\tau}}\right) \\ & + E_0 \left[\operatorname{erfc}\left(\frac{\Lambda_1 x}{\sqrt{4\tau}}\right) - U(x, \tau; b_e, C_e) \right] \\ & + E_0^* \left[\operatorname{erfc}\left(\frac{\Lambda_1 x}{\sqrt{4\tau}}\right) - e^{-\zeta_w x} U(x, \tau; b_w, C_w) \right] + o(\tau^{-1/2}) \end{aligned} \quad (3.4.1)$$

$$P(x, \tau) \sim \frac{\gamma h C_e}{\Lambda_1} U(x, \tau; b_e, C_e) + o(\tau^{-1/2}) \quad (3.4.2)$$

$$u(x, \tau) \sim \frac{h}{\Lambda_1} \left[U(x, \tau; b_e, C_e) - \operatorname{erfc}\left(\frac{\Lambda_1 x}{\sqrt{4\tau}}\right) \right] + o(\tau^{-1/2}) \quad (3.4.3)$$

$$\begin{aligned} \frac{Y_X(x, \tau)}{X W_X} \sim & \frac{(\beta_T - \beta_\rho) h}{E_1} \left[\sqrt{\frac{4\tau}{\pi}} \exp\left[-\frac{\Lambda_1^2 x^2}{4\tau}\right] - \Lambda_1 x \operatorname{erfc}\left(\frac{\Lambda_1 x}{\sqrt{4\tau}}\right) \right. \\ & \left. - \frac{\Lambda_1}{\zeta_w} \exp(-\zeta_w x) U(x, \tau; b_w, C_w) \right] + o(\tau^{-1/2}) \end{aligned} \quad (3.4.4)$$

where

$$U(x, \tau; b, C) \equiv 1/2 \left[\operatorname{erfc} \left\{ \frac{b(x/C - \tau)}{\sqrt{\tau}} \right\} + e^{4b^2 x/C} \operatorname{erfc} \left\{ \frac{b(x/C + \tau)}{\sqrt{\tau}} \right\} \right] \quad (3.4.5)$$

The characteristic picture of the wave function $U(x, \tau; b, C)$ is shown in Fig. 3.5. It is observed that the wave front travels with the speed of C and spreads out like the square-root of time. The complex processes are essentially the same as for the previous case both of which are composed of diffusive waves and a boundary layer adjacent to the hot-surface. In the latter case, we get a nonstationary reaction zone with a continuous supply of heat from the bounding surface. The dimensionless thermal flux from the wall $q_0 = \Lambda_1$ is determined from the first group of terms in (3.4.1), which is a solution of the linear heat conduction problem. The associated perturbation temperature, velocity, and species concentration of oxidant are plotted as function of $x^* = x/\tau$ in Figs. 3.6-3.8 at different instants in time. In contrast to the case when the surface temperature does not vary with time, there are no relatively maximum perturbations in the field. We could attribute this difference to the fact that the case of constant surface temperature provides a more intensive heat supply from an outer source. For instance, when the combustible mixture ignited by a similar heat impulse, the time of heating action is shorter for the case of constant surface temperature than for that of constant heat flow.

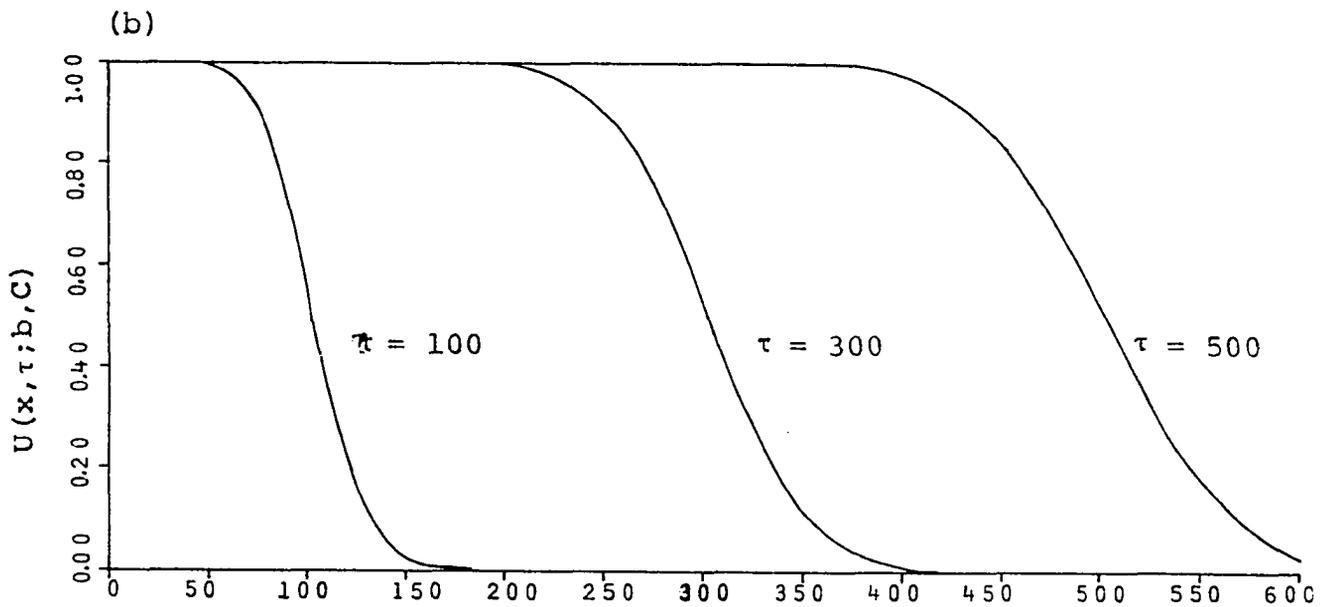
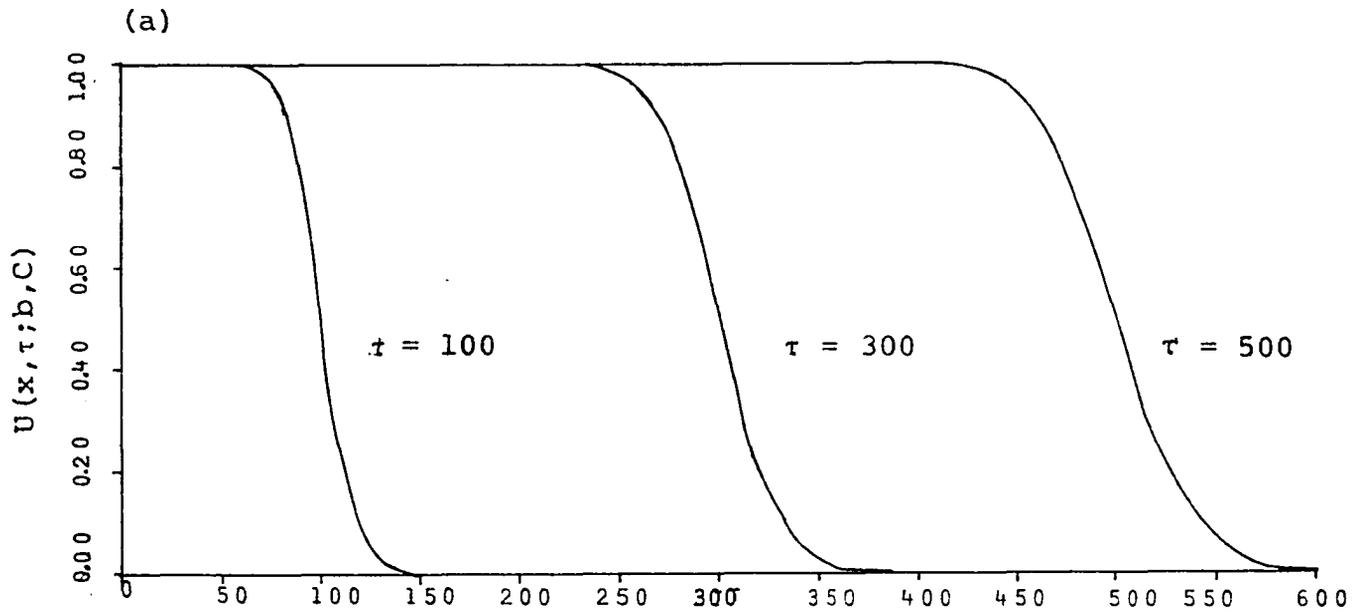


Figure 3.5 Diffusive Wave Behavior of Function $U(x, \tau; b, C)$:
(a) $b=0.5, C=1.0$; (b) $b=0.3, C=1.0$

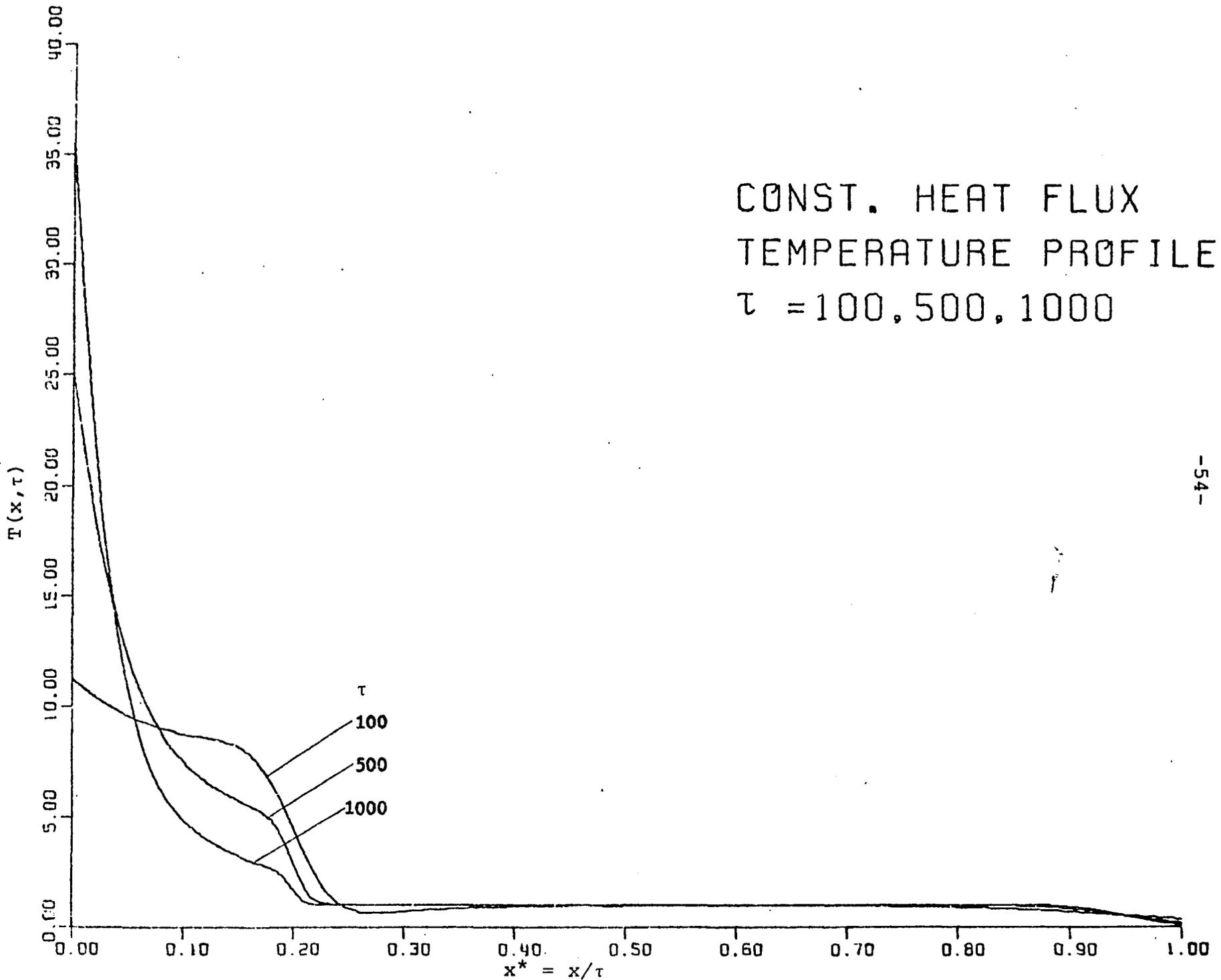


Figure 3.6 Long-time Behavior of the Temperature Perturbation for Ignition of Gases by a Constant Heat Flow

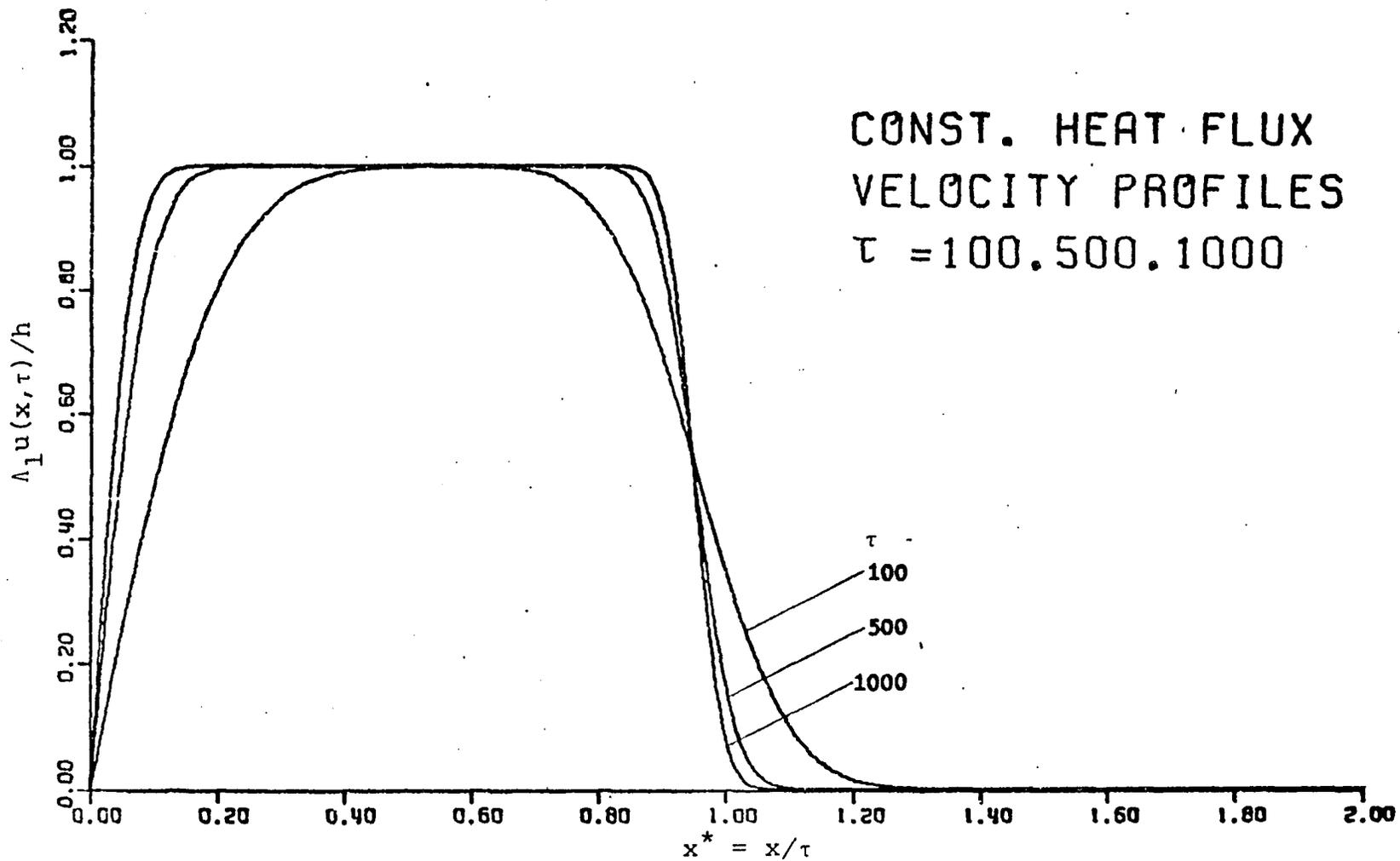


Figure 3.7 Long-time Behavior of the Velocity Perturbation for Ignition of Gases by a Constant Heat Flow

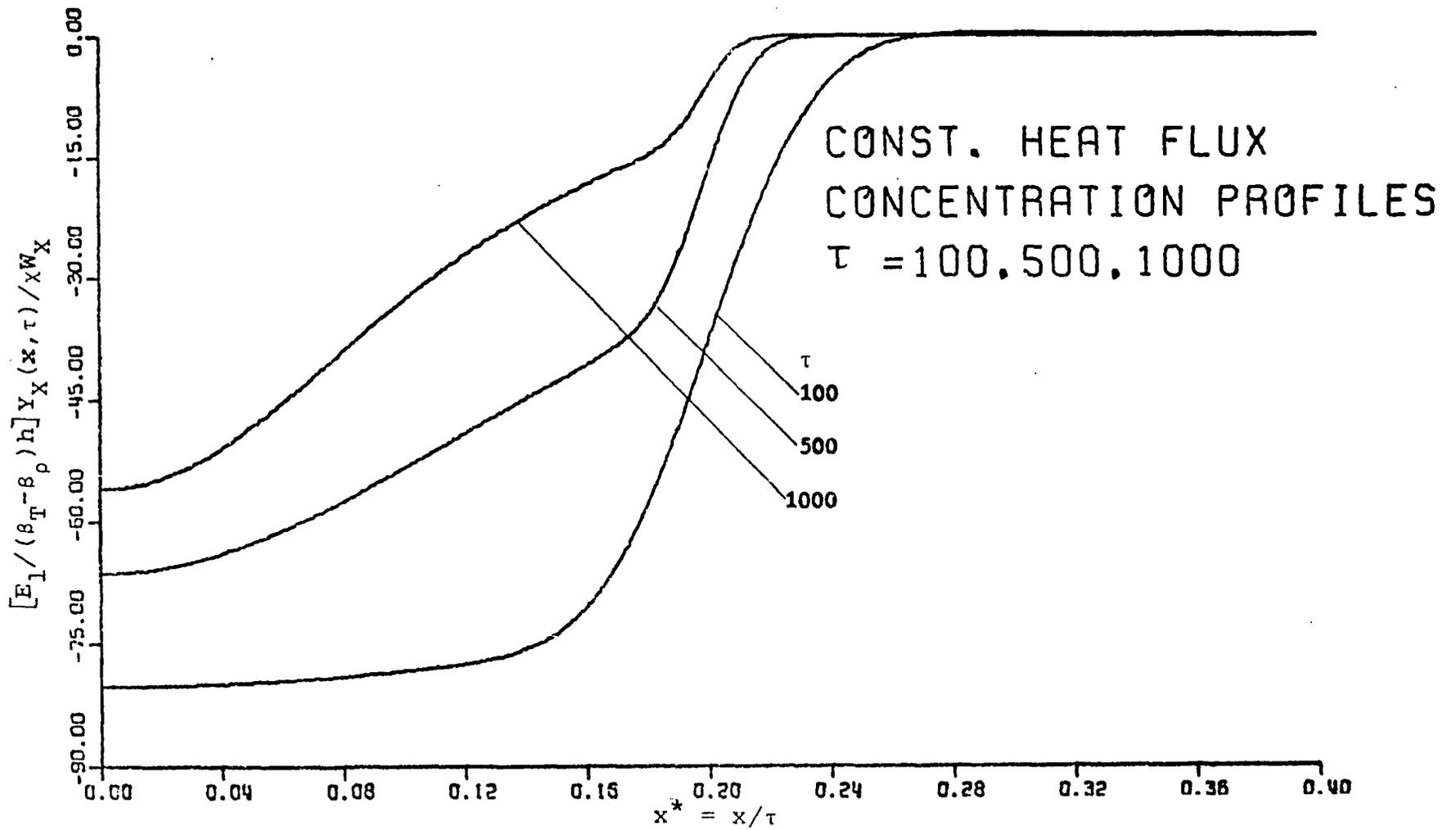


Figure 3.8 Long-time Behavior of the Species Concentration of Oxidant for Ignition of Gases by a Constant Heat Flow

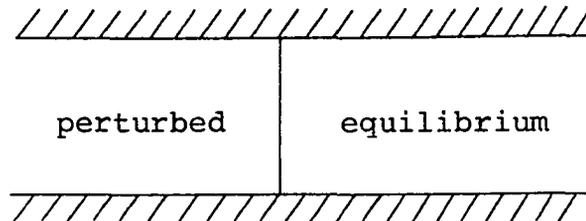
The damping term $\exp(-\zeta_w x)$ associated with the chemical reaction exists in both cases, since the heat flux into the burning zone decreases as the flame front moves away from the hot surface. However, the induced perturbations do not die out with time for the case of constant heat flux, because there is a constant supply of heat from the bounding surface.

CHAPTER IV

APPLICATION TO EXPLOSION PROBLEM

4.1 Description of the Problem

The one-dimensional explosion problem will be considered in this chapter. The problem is envisaged as follows. Initially, a planar diaphragm at $x = 0$ separates two semi-infinite regions. On the right-hand side of the diaphragm, $x > 0$, the mixture of oxidant, fuel and product is in equilibrium with pressure, P_0 , density, ρ_0 , temperature, T_0 , and mass species fractions Y_{α_0} , $\alpha = X, F,$ and P . On the left-hand side of the diaphragm, $x < 0$, the conditions are perturbed from the right-hand side by small amounts and may or may not be in chemical equilibrium. The perturbations are denoted by the symbol Δ with the appropriate subscripts, as indicated in Fig. 4.1.



$x < 0, t < 0$	$x > 0, t < 0$
$P = P_0(1 + \Delta_P)$	$P = P_0$
$\rho = \rho_0(1 + \Delta_\rho)$	$\rho = \rho_0$
$T = T_0(1 + \Delta_T)$	$T = T_0$
$Y_X = Y_{X_0} + \Delta_X$	$Y_X = Y_{X_0}$
$Y_F = Y_{F_0} + \Delta_F$	$Y_F = Y_{F_0}$
$Y_P = 1 - Y_{X_0} - Y_{F_0} - \Delta_X - \Delta_F$	$Y_P = 1 - Y_{X_0} - Y_{F_0}$

Fig. 4.1 Configuration for One-Dimensional
Explosion Problem

The initial perturbations are not all independent, they are related by the equation

$$\Delta_P = \Delta_\rho + \Delta_T + \alpha_X \Delta_X + \alpha_F \Delta_F$$

At a given instant $t = 0$, the diaphragm is withdrawn instantaneously. The thermal regime of the gas mixture is then determined at subsequent instants. The problem then is to solve the governing equation (A.7) subject to the above initial conditions and the requirement that all perturbations vanish at infinity.

This problem could be considered as a simplified model of a soap-bubble explosion where hot burned gas is introduced into an infinite space occupied by a fuel gas mixture and ignites the surrounding unburned gas.

4.2 Laplace-Transform Analysis

The diffusion equation $D_S J = 0$ can be solved separately. The initial conditions are $J(x < 0, 0) = \Delta$ and $J(x > 0, 0) = 0$, where $\Delta = \Delta_F - \sigma \Delta_X$ is a mixture strength parameter. Further, J is continuous at $x = 0$. The result is:

$$J(x, \tau) / \Delta = (1/2) \operatorname{erfc} \left(\frac{\sqrt{S_c} x}{\sqrt{4\tau}} \right) \quad (4.2.1)$$

Therefore, the species concentration of fuel, Y_F is defined in terms of that of the oxidant, Y_X , and $J(x, \tau)$. Hence, it is only necessary to solve for the species concentration of the oxidant among the species. With J known, equation (A.7) constitutes a seventh order non-homogeneous equation for ϕ . If a Laplace transformation with respect to time is applied to equation (A.7), the following differential equation is obtained

$$\delta_1 \frac{\partial^6 \bar{\phi}}{\partial x^6} + \delta_2 \frac{\partial^4 \bar{\phi}}{\partial x^4} + \delta_3 \frac{\partial^2 \bar{\phi}}{\partial x^2} - \delta_4 \bar{\phi} = \psi(x, s) \quad (4.2.2)$$

where

$$\psi(x < 0, s) = \delta_4 \Delta_P / \gamma s^2 - (1/2) \Delta S_c (\alpha_F E_1 - A_F E_3) (P_r - S_c) s e^{\sqrt{S_c} s x} \quad (4.2.3)$$

$$\psi(x > 0, s) = (1/2) \Delta S_c (\alpha_F E_1 - A_F E_3) (P_r - S_c) s e^{-\sqrt{S_c} s x} \quad (4.2.4)$$

and $\delta_1, \delta_2, \delta_3$, and δ_4 are defined as

$$\begin{aligned}
 \delta_1 &= \gamma s + 1 \\
 \delta_2 &= \alpha s^2 - \beta_2 s - \beta_4 \\
 \delta_3 &= \beta_1 s^3 + (P_r S_c + \beta_3) s^2 + P_r S_c \left[E_1 + (\beta_T - \beta \rho) (Q - E_3) \right] s \\
 \delta_4 &= P_r S_c \left[s^4 + \{ E_1 + \gamma \beta_T (Q - E_3) \} s^3 \right]
 \end{aligned} \tag{4.2.5}$$

The general solutions of equation (4.2.2) can be found in the form

$$\begin{aligned}
 \bar{\phi}(x > 0, s) &= A_1^+ e^{-\lambda_1 x} + A_3^+ e^{-\lambda_3 x} + A_4^+ e^{-\lambda_4 x} \\
 &\quad + \frac{(\alpha_F E_1 - A_F E_3) (P_r - S_c)}{2K} e^{-\sqrt{S_c} s x}
 \end{aligned} \tag{4.2.6}$$

$$\begin{aligned}
 \bar{\phi}(x < 0, s) &= A_1^- e^{\lambda_1 x} + A_3^- e^{\lambda_3 x} + A_4^- e^{\lambda_4 x} \\
 &\quad - \frac{(\alpha_F E_1 - A_F E_3) (P_r - S_c)}{2K} e^{\sqrt{S_c} s x} - \Delta_P / \gamma s^2
 \end{aligned} \tag{4.2.7}$$

where A_1^\pm , A_3^\pm , and A_4^\pm are constants of integration and where

$$K \equiv \delta_1 S_c^2 s^2 + \delta_2 S_c s + \delta_3 - \delta_4 / S_c s \tag{4.2.8}$$

In the limit of $s \rightarrow 0$, corresponding to large time, we have asymptotic expansion for K in the form

$$K \sim S_c s (P_r - S_c) [E_1 - (\beta_T - \beta \rho) E_3] + O(s^2) \tag{4.2.9}$$

and λ_1 , λ_3 , and λ_4 are the same as presented in Chapter II, equation (2.4.3) without taking account of pressure diffusion

and multicomponent diffusion. The constants A_1^+ , A_3^+ , and A_4^+ are determined by requiring that \bar{u} , \bar{P} , $\bar{\rho}$, \bar{Y}_X , $(\bar{Y}_X)_x$ and \bar{T}_x be continuous at $x = 0$. The large-time expansions of these constants are found to be

$$\begin{aligned} A_1^- &\sim \Lambda_1^*/s + 0(1) \\ A_3^- &\sim \Delta_P/2\gamma s^2 + 0(1/s) \\ A_4^- &\sim \Lambda_4^* + 0(s) \end{aligned} \quad (4.2.10)$$

and

$$\begin{aligned} A_1^+ &= -A_1^- \\ A_3^+ &= -A_3^- \\ A_4^+ &= -A_4^- \end{aligned} \quad (4.2.11)$$

where

$$\begin{aligned} \Lambda_1^* &= \frac{h_1}{2\Lambda_1} \left[\frac{\Delta_P}{C_e^2} + \beta_T \Delta_P + \frac{E_1 \Delta_\rho}{P_\gamma Q - S_c E_3} \right. \\ &\quad \left. + \Delta h_2/h_1 + A_X \Delta_X + A_F \Delta_F \right] \end{aligned} \quad (4.2.12)$$

$$\Lambda_4^* = \frac{h_1}{2\zeta_w} \left[(\beta_T - \beta\rho) \Delta_\rho - \beta_T \Delta_P + (A_X \Delta_X + A_F \Delta_F) \right] \quad (4.2.13)$$

$$h_1 = \frac{P_\gamma Q - S_c E_3}{E_1 + (\beta_T - \beta\rho)(P_\gamma Q - S_c E_3)} \quad (4.2.14)$$

$$h_2 = \frac{\alpha_F E_1 - A_F E_3}{E_1 - (\beta_T - \beta\rho) E_3} \quad (4.2.15)$$

with these results the approximate transforms of the velocity, pressure, species concentration of oxidant, and temperature, valid for small values of transform variable, can be written as

$$\begin{aligned} \bar{u}(x,s) \sim \Lambda_1 \Lambda_1^* \frac{e^{-\sqrt{s}\Lambda_1 x}}{\sqrt{s}} + \frac{\Delta_p}{2\gamma C_e} \frac{e^{-\lambda_3 x}}{s} \\ + \zeta_w \Lambda_4^* e^{-\lambda_4 x} - \frac{\Delta h_2}{2\sqrt{s} C_e} \frac{e^{-\sqrt{s} C_e s x}}{\sqrt{s}} \end{aligned} \quad (4.2.16)$$

$$\begin{aligned} \bar{P}(x \geq 0, s) \sim -\gamma(\Lambda_1^2 - 1) \Lambda_1^* e^{-\sqrt{s}\Lambda_1 x} - \frac{\Delta_p}{2C_e^2} e^{-\lambda_3 x} + \frac{\Delta_p}{2s} e^{-\lambda_3 x} \\ - \gamma \zeta_w^2 \Lambda_4^* e^{-\lambda_4 x} + \frac{\gamma(S_c - 1)\Delta h_2}{2S_c} e^{-\sqrt{s} C_e s x} \end{aligned} \quad (4.2.17)$$

$$\begin{aligned} \bar{P}(x \leq 0, s) \sim \gamma(\Lambda_1^2 - 1) \Lambda_1^* e^{\sqrt{s}\Lambda_1 x} + \frac{\Delta_p}{2C_e^2} e^{\lambda_3 x} - \frac{\Delta_p}{2s} e^{\lambda_3 x} \\ + \gamma \zeta_w^2 \Lambda_4^* e^{\lambda_4 x} + \frac{\Delta_p}{s} - \frac{\gamma(S_c - 1)\Delta h_2}{2S_c} e^{\sqrt{s} C_e s x} \end{aligned} \quad (4.2.18)$$

$$\begin{aligned} \frac{\bar{Y}_X}{XW_X}(x \geq 0, s) \sim \frac{-(\beta_T - \beta_\rho) \Lambda_1^2 \Lambda_1^*}{E_1} \frac{e^{-\sqrt{s}\Lambda_1 x}}{s} - \frac{\left(\frac{\beta_T - \beta_\rho}{C_e^2} - \gamma \beta_T \right) \Delta_p}{2\gamma E_1} \frac{e^{-\lambda_3 x}}{s} \\ + \frac{\zeta_w^2 \Lambda_4^*}{P_r Q - S_c E_3} \frac{e^{-\lambda_4 x}}{s} - \frac{\Delta}{2E_1} \left[A_F - (\beta_T - \beta_\rho) h_2 \right] \frac{e^{-\sqrt{s} C_e s x}}{s} \end{aligned} \quad (4.2.19)$$

$$\begin{aligned} \frac{\bar{Y}_X}{XW_X}(x \leq 0, s) \sim \frac{(\beta_T - \beta_\rho) \Lambda_1^2 \Lambda_1^*}{E_1} \frac{e^{\sqrt{s}\Lambda_1 x}}{s} + \frac{\left(\frac{\beta_T - \beta_\rho}{C_e^2} - \gamma \beta_T \right) \Delta_p}{2\gamma E_1} \frac{e^{\lambda_3 x}}{s} + \frac{\Delta}{XW_X} \frac{1}{s} \\ - \frac{\zeta_w^2 \Lambda_4^*}{P_r Q - S_c E_3} \frac{e^{\lambda_4 x}}{s} + \frac{\Delta}{2E_1} \left[A_F - (\beta_T - \beta_\rho) h_2 \right] \frac{e^{\sqrt{s} C_e s x}}{s} \end{aligned} \quad (4.2.20)$$

$$\begin{aligned}
 T(x \geq 0, s) \sim & - \frac{\Lambda_1^2 \Lambda_1^*}{h} \frac{e^{-\sqrt{s} \Lambda_1 x}}{s} - \frac{\Delta_p}{2\gamma} \beta_3^* \frac{e^{-\lambda_3 x}}{s} \\
 & - \frac{(P_r Q) \zeta_w^2 \Lambda_4^*}{P_r Q - S_c E_3} \frac{e^{-\lambda_4 x}}{s} + \frac{\gamma (S_c - 1) \Delta h_2}{2S_c} e^{-\sqrt{S_c} s x}
 \end{aligned} \tag{4.2.21}$$

$$\begin{aligned}
 T(x \leq 0, s) \sim & \frac{\Lambda_1^2 \Lambda_1^*}{h} \frac{e^{\sqrt{s} \Lambda_1 x}}{s} + \frac{\Delta_p}{2\gamma} \beta_3^* \frac{e^{\lambda_3 x}}{s} \\
 & + \frac{(P_r Q) \zeta_w^2 \Lambda_4^*}{P_r Q - S_c E_3} \frac{e^{\lambda_4 x}}{s} - \frac{\gamma (S_c - 1) \Delta h_2}{2S_c} e^{\sqrt{S_c} s x} \\
 & + (\Delta_p - \Delta_\rho - \alpha_X \Delta_X - \alpha_F \Delta_F) / s
 \end{aligned} \tag{4.2.22}$$

where

$$\beta_3^* = \frac{1}{C_e^2} - \gamma - \frac{E_3 (\beta_T - \beta_\rho - \gamma \beta_T)}{E_1 + (\beta_T - \beta_\rho) (Q - E_3)} \tag{4.2.23}$$

4.3 Asymptotic Approximations for Large Time

The inversion of the transformed field variables found in the previous section can be accomplished by means of standard Laplace-transform tables and by the approximation method proposed by Rasmussen [22]. The large-time approximation for the velocity field is

$$\begin{aligned}
 u(x, \tau) \sim & \Lambda_1 \Lambda_1^* \frac{e^{-\Lambda_1^2 x^2 / 4\tau}}{\sqrt{\pi\tau}} - \frac{\Delta h_2}{2\sqrt{S_c}} \frac{e^{-S_c x^2 / 4\tau}}{\sqrt{\pi\tau}} + \zeta_w \Lambda_3^* e^{-\zeta_w |x|} G(|x|, \tau; b, C) \\
 & + \frac{\Delta_p}{2\gamma C_e} U(|x|, \tau; b_e, C_e)
 \end{aligned} \tag{4.3.1}$$

where

$$G(|x|, \tau; b, C) \equiv \frac{b_w |x|}{C_w} \frac{e^{-b_w^2 (\tau - x/C_w)^2 / \tau}}{\sqrt{\pi\tau}} \tag{4.3.2}$$

The contribution associated with the initial pressure differential $\Delta_p U(|x|, \tau; b_e, C_e) / 2\gamma C_e$ is dominant and corresponds to the compression wave in one direction and an expansion wave in the other. The resulting pressure distribution is quite like that in Figure 3.1. The first two terms in equation (4.3.1) describe the diffusive-type relaxation of the initial disturbance caused by the removal of the diaphragm. The disturbance at $x = 0$ dies out like $\tau^{-1/2}$. The higher-order contribution is given in the third term in equation (4.3.1), which is generated by chemical reaction. They constitute a compression wave traveling in one direction and an expansion wave traveling in the other. This effect behaves as a pulse, centered at $x = C_w \tau$ and traveling with the laminar flame speed C_w , and dies out approximately like $\tau^{-3/2}$. The corresponding large-time approximation for the pressure is

$$\begin{aligned}
 P(x \geq 0, \tau) \sim & -\gamma(\Lambda_1^2 - 1)\Lambda_1^* \frac{\Lambda_1 x}{\sqrt{4\pi\tau^3}} e^{-\Lambda_1^2 x^2 / 4\tau} + \frac{\gamma(S_c - 1)\Delta h_2}{2S_c} \frac{\sqrt{S_c} x}{\sqrt{4\pi\tau^3}} e^{-S_c x^2 / 4\tau} \\
 & - \frac{\Delta_p}{2C_e^2} G(|x|, \tau; b_e, C_e) + \Delta_p U(|x|, \tau; b_e, C_e) / 2 \\
 & - \gamma\zeta_w^2 \Lambda_4^* e^{-\zeta_w x} G(|x|, \tau; b_w, C_w) \tag{4.3.3}
 \end{aligned}$$

$$\begin{aligned}
 P(x \leq 0, \tau) \sim & -\gamma(\Lambda_1^2 - 1)\Lambda_1^* \frac{\Lambda_1 x}{\sqrt{4\pi\tau^3}} e^{-\Lambda_1^2 x^2 / 4\tau} + \frac{\gamma(S_c - 1)\Delta h_2}{2S_c} \frac{\sqrt{S_c} x}{\sqrt{4\pi\tau^3}} e^{-S_c x^2 / 4\tau} \\
 & + \frac{\Delta_p}{2C_e^2} G(x, \tau; b_e, C_e) - \Delta_p U(|x|, \tau; b_e, C_e) / 2 + \Delta_p \\
 & + \gamma\zeta_w^2 \Lambda_4^* e^{\zeta_w x} G(|x|, \tau; b_w, C_w) \tag{4.3.4}
 \end{aligned}$$

The functions associated with initial pressure perturbation $\Delta_p U(x, \tau; b_e, C_e)/2$ dominate the pressure distribution. The other contributions die out at least as fast as $\tau^{-1/2}$. The variation of pressure generated by the flame propagation is described by the functions $G(|x|, \tau; b_w, C_w)$ and a damping term $e^{-\zeta_w x}$. When the initial pressure perturbation across the diaphragm Δ_p vanishes, this combustion wave becomes the dominating disturbance. The large-time approximation for the species concentration of oxidant is

$$\begin{aligned} \frac{Y_X}{XW_X}(x \geq 0, \tau) \sim & - \frac{(\beta_T - \beta_\rho) \Lambda_1^2 \Lambda_1^*}{E_1} \operatorname{erfc} \left(\frac{\Lambda_1 x}{\sqrt{4\tau}} \right) - \frac{\Delta}{2E_1} \left[A_F - (\beta_T - \beta_\rho) h_2 \right] \operatorname{erfc} \left(\frac{\sqrt{S_c} x}{\sqrt{4\tau}} \right) \\ & - \frac{(\beta_T - \beta_\rho - \gamma C_e^2 \beta_T) \Delta_p}{2\gamma C_e^2 E_1} U(|x|, \tau; b_e, C_e) \\ & + \frac{\zeta_w^2 \Lambda_1^*}{P Q - S_c E_3} e^{-\zeta_w x} U(|x|, \tau; b_w, C_w) \end{aligned} \quad (4.3.5)$$

$$\begin{aligned} \frac{Y_X}{XW_X}(x \leq 0, \tau) \sim & \frac{(\beta_T - \beta_\rho) \Lambda_1^2 \Lambda_1^*}{E_1} \operatorname{erfc} \left(\frac{-\Lambda_1 x}{\sqrt{4\tau}} \right) + \frac{\Delta}{2E_1} \left[A_F - (\beta_T - \beta_\rho) h_2 \right] \operatorname{erfc} \left(\frac{-\sqrt{S_c} x}{\sqrt{4\tau}} \right) \\ & + \frac{\Delta_X}{XW_X} + \frac{(\beta_T - \beta_\rho - \gamma C_e^2 \beta_T) \Delta_p}{2\gamma C_e^2 E_1} U(|x|, \tau; b_e, C_e) \\ & - \frac{\zeta_w^2 \Lambda_1^*}{P Q - S_c E_3} e^{\zeta_w x} U(|x|, \tau; b_w, C_w) \end{aligned} \quad (4.3.6)$$

The asymptotic solutions show that the species concentration of oxidant are influenced by initial pressure perturbation and chemical non-equilibrium, besides the diffusive-type re-

laxation of initial mass fraction perturbation. Without chemistry and Δ_p , the solution exhibits entirely diffusive behavior as that of inert binary mixture. With the known asymptotic behaviour of oxidant, the solution for mass fraction of fuel can be found from equation (4.2.1).

The large-time approximation for the temperature field is

$$\begin{aligned}
 T(x \geq 0, \tau) \sim & - \frac{\Lambda_1^2 \Lambda_1^*}{h} \operatorname{erfc} \left(\frac{\Lambda_1 x}{\sqrt{4\tau}} \right) + \frac{\gamma (S_c - 1) h_2}{2S_c} \frac{\sqrt{S_c} x}{\sqrt{4\pi\tau}^3} e^{-S_c x^2/4\tau} \\
 & - \frac{\beta_3 \Delta_p}{2\gamma} U(|x|, \tau; b_e, C_e) \\
 & - \frac{(P_\gamma Q) \zeta_w^2 \Lambda_1^*}{P_\gamma Q - S_c E_3} e^{-\zeta_w x} U(|x|, \tau; b_w, C_w) \quad (4.3.7)
 \end{aligned}$$

$$\begin{aligned}
 T(x \leq 0, \tau) \sim & \Delta_T + \frac{\Lambda_1^2 \Lambda_1^*}{h} \operatorname{erfc} \left(\frac{\Lambda_1 x}{\sqrt{4\tau}} \right) + \frac{\gamma (S_c - 1) h_2}{2S_c} \frac{\sqrt{S_c} x}{\sqrt{4\pi\tau}^3} e^{-S_c x^2/4\tau} \\
 & + \frac{\beta_3 \Delta_p}{2\gamma} U(|x|, \tau; b_e, C_e) \\
 & + \frac{(P_\gamma Q) \zeta_w^2 \Lambda_1^*}{P_\gamma Q - S_c E_3} e^{\zeta_w x} U(|x|, \tau; b_w, C_w) \quad (4.3.8)
 \end{aligned}$$

It is noted from the above results that the flame propagation provides an important contribution to the temperature field, as is evident from the last terms in equation (4.3.7) and (4.3.8). This contribution is proportional to the effective heat released by combustion, Q . The terms associated with wave function $U(|x|, \tau; b_e, C_e)$ are proportional to Δ_p , hence they are of gas-dynamic origin. The first two terms in (4.3.7) and (4.3.8) are

associated with classical thermal conduction and mass diffusion. When Schmidt number is unity, the contribution of mass diffusion to the temperature variation vanishes.

The above results show that the shock wave front is centered at $x = C_e \tau$ and diffuses with a characteristic diffusion width defined by

$$x - C_e \tau = \tau^{1/2} / b_e \quad (4.3.9)$$

Thus the linearized theory predicts a shock wave with a diffusion width increasing indefinitely with time like $\sqrt{\tau}$. This leads to an estimate of the time at which the linear solution breaks down. As is expected, the thickness of a weak shock in the steady flow is of the order of $1/\Delta$, where Δ is the initial perturbation. Since we expect the solution of the shock tube problem to yield a steady-state shock as $\tau \rightarrow \infty$, we conclude that the linearized solution becomes invalid when $\tau = O(1/\Delta^2)$. This nonuniformity will be treated in the next chapter by method of multiple scales [41,42].

CHAPTER V

NONLINEAR INTERACTION

For very long times, the wave fronts in linearized theory are dominated by transport diffusive effects. It is known in shock-wave behavior, however, that diffusive and nonlinear effects tend to counteract each other. In order to delineate the balance between the diffusive linear terms and the steepening nonlinear terms, let us isolate the viscosity by means of the dimensionless parameter

$$\epsilon \equiv \frac{\tilde{\mu}_0}{\rho_0 a_{f_0} L} \quad (5.1.1)$$

where L is some characteristic length pertinent to a given problem. The parameter ϵ is to be regarded as small so that the transport terms can be balanced with the nonlinear terms, which are also small. The Prandtl and Schmidt numbers are of order unity. Let us introduce new independent variables such that

$$\tilde{\tau} = \frac{a_{f_0} t}{L} = \epsilon \tau \quad \text{and} \quad \tilde{\mathbf{r}} = \frac{\mathbf{r}}{L} = \epsilon \mathbf{r} \quad (5.1.2)$$

It follows in the new variables that $\nabla = \epsilon \tilde{\nabla}$ and $\vec{\nabla} = \epsilon \tilde{\nabla} \phi$.

In the new variables, the old n th order derivatives in both

space and time now become proportional to ϵ^n . Thus we can rewrite the governing potential equation, equation (2.3.18), and display the lowest two orders as

$$\left[C_e^{2\hat{V}^2} \phi - \phi_{\hat{\tau}\hat{\tau}} \right]_{\hat{\tau}} = + \frac{\epsilon}{A_4} \left[A_5 \hat{V}^4 \phi - B_5 \hat{V}^2 \phi_{\hat{\tau}\hat{\tau}} + P_r S_C^2 \phi_{\hat{\tau}\hat{\tau}\hat{\tau}\hat{\tau}} \right] + 0(\epsilon^2) \quad (5.1.3)$$

The lowest-order terms thus constitute the classical wave operator with the equilibrium speed of sound. The diffusive transport terms enter as a first-order correction involving derivatives of one-higher order. The nonlinear terms, which were omitted by the original linearization, should also appear to order ϵ in equation (5.1.3).

To obtain the lowest order nonlinear correction, we return to the original equations, omit the transport terms for simplicity since they are already accounted for in (5.1.3), but retain the lowest order nonlinear terms. We replace the perturbation variables in (2.2.1) by $\rho' = \epsilon \hat{\rho}$, and so on for the other primed variables, and utilize the normalizations (5.1.2). The governing equations then become

$$\frac{\partial \hat{\rho}}{\partial \hat{\tau}} + \hat{V} \cdot \hat{V} + \epsilon \hat{V} \cdot (\hat{\rho} \hat{V}) = 0 \quad (5.1.4)$$

$$\frac{\partial \hat{V}}{\partial \hat{\tau}} + (1/\gamma) \hat{V} \hat{P} + \epsilon \left[\hat{\rho} \frac{\partial \hat{V}}{\partial \hat{\tau}} + \hat{V} (\hat{V}^2/2) \right] + 0(\epsilon^2) = 0 \quad (5.1.5)$$

$$\begin{aligned} \frac{\partial \hat{T}}{\partial \hat{\tau}} + Q \frac{\partial (\hat{V}_X / \chi W_X)}{\partial \hat{\tau}} - \frac{\gamma-1}{\gamma} \frac{\partial \hat{P}}{\partial \hat{\tau}} + \epsilon \left[\frac{\gamma-1}{\gamma} \hat{\rho} \frac{\partial \hat{P}}{\partial \hat{\tau}} \right. \\ \left. + \epsilon_1 \frac{\partial}{\partial \hat{\tau}} \left(\hat{T} \frac{\hat{V}_X}{\chi W_X} \right) + \frac{T_0}{C_{P_0}} \left(\frac{\partial C_P}{\partial T} \right)_0 \hat{T} \frac{\partial \hat{T}}{\partial \hat{\tau}} \right] + 0(\epsilon^2) = 0 \end{aligned} \quad (5.1.6)$$

$$A(\tilde{Y}_X/\chi W_X) - \beta_\rho \tilde{\rho} - \beta_T \tilde{T} + \epsilon \left[\frac{\partial(\tilde{Y}_X/\chi W_X)}{\partial \tilde{\tau}} + \tilde{R}_1 \right] + 0(\epsilon^2) = 0 \quad (5.1.7)$$

$$\tilde{P} = \tilde{\rho} + \tilde{T} + E_3(\tilde{Y}_X/\chi W_X) + \epsilon \left[\tilde{\rho} \tilde{T} + E_3(\tilde{Y}_X/\chi W_X)(\tilde{\rho} + \tilde{T}) \right] + 0(\epsilon^2) \quad (5.1.8)$$

where

$$\epsilon_1 \equiv \frac{(C_{P,O,X} - C_{P,O,P})\chi W_X + (C_{P,O,F} - C_{P,O,P})fW_F}{C_{P,O}} \quad (5.1.9)$$

$$\left(\frac{\partial C_P}{\partial T} \right)_O \equiv Y_{X,O} \left[\frac{\partial}{\partial T} (C_{P,X} - C_{P,P}) \right]_O + Y_{F,O} \left[\frac{\partial}{\partial T} (C_{P,F} - C_{P,P}) \right]_O + \left(\frac{\partial C_{P,P}}{\partial T} \right)_O \quad (5.1.10)$$

$$\begin{aligned} \tilde{R}_1 \equiv & \left(\frac{\partial^2 R}{\partial \rho^2} \right)_O \rho_O^2 \frac{\tilde{\rho}^2}{2} + \left(\frac{\partial^2 R}{\partial T^2} \right)_O T_O^2 \frac{\tilde{T}^2}{2} + \left(\frac{\partial^2 R}{\partial Y_X^2} \right)_O \frac{\tilde{Y}_X^2}{2} + \left(\frac{\partial^2 R}{\partial Y_F^2} \right)_O \frac{\tilde{Y}_F^2}{2} \\ & + \left(\frac{\partial^2 R}{\partial \rho \partial Y_X} \right)_O \rho_O \tilde{\rho} \tilde{Y}_X + \left(\frac{\partial^2 R}{\partial \rho \partial Y_F} \right)_O \rho_O \tilde{\rho} \tilde{Y}_F + \left(\frac{\partial^2 R}{\partial \rho \partial T} \right)_O \rho_O T_O \tilde{\rho} \tilde{T} \\ & + \left(\frac{\partial^2 R}{\partial T \partial Y_X} \right)_O T_O \tilde{T} \tilde{Y}_X + \left(\frac{\partial^2 R}{\partial T \partial Y_F} \right)_O T_O \tilde{T} \tilde{Y}_F + \left(\frac{\partial^2 R}{\partial Y_X \partial Y_F} \right)_O \tilde{Y}_X \tilde{Y}_F \end{aligned} \quad (5.1.11)$$

$$A \equiv E_1 - \beta_T E_3 \quad (5.1.12)$$

These equations can be manipulated so that the following equation for the perturbation potential is obtained to the lowest two orders:

$$C_e^{2\gamma} \nabla^2 \phi - \phi_{\tau\tau} = \epsilon \left[\frac{\partial}{\partial \tau} (\nabla \phi)^2 + \zeta^* \phi_{\tau} \nabla^2 \phi + \zeta_O^* \phi_{\tau\tau\tau} \right] + O(\epsilon^2) \quad (5.1.13)$$

where

$$\zeta^* \equiv C_e^4 \{ 2 [E_1 + \beta_T (Q - E_3)] (\zeta_T / C_e^2 + E_3 \zeta_O / C_e^2 + E_3 \zeta_O \zeta_T) + (Q - E_3) \zeta_R - E_1 \zeta_C \} / [E_1 + (\beta_T - \beta_\rho) (Q - E_3)] \quad (5.1.14)$$

$$\zeta_O^* \equiv C_e^2 \zeta_O / [E_1 + (\beta_T - \beta_\rho) (Q - E_3)] \quad (5.1.15)$$

$$\begin{aligned} \zeta_R \equiv & \left(\frac{\partial^2 R}{\partial \rho^2} \right)_O \frac{\rho_O^2}{C_e^4} + \left(\frac{\partial^2 R}{\partial T^2} \right)_O T_O^2 \zeta_T^2 + \left[\left(\frac{\partial^2 R}{\partial Y_X^2} \right)_O + \left(\frac{\partial^2 R}{\partial Y_F^2} \right)_O \right] \left[1 + \left(\frac{fW_F}{\chi W_X} \right)^2 \right] \zeta_O^2 \\ & + \left[\left(\frac{\partial^2 R}{\partial \rho \partial Y_X} \right)_O + \left(\frac{\partial^2 R}{\partial \rho \partial Y_F} \right)_O \right] \left(1 + \frac{fW_F}{\chi W_X} \right) \frac{\rho_O \zeta_O}{C_e^2} + \left(\frac{\partial^2 R}{\partial \rho \partial T} \right)_O \frac{\rho_O T_O \zeta_T}{C_e^2} \\ & + \left[\left(\frac{\partial^2 R}{\partial T \partial Y_X} \right)_O + \left(\frac{\partial^2 R}{\partial T \partial Y_F} \right)_O \right] \left(1 + \frac{fW_F}{\chi W_X} \right) T_O \zeta_T \zeta_O + \left(\frac{\partial^2 R}{\partial Y_X \partial Y_F} \right)_O \frac{fW_F}{\chi W_X} \zeta_O^2 \end{aligned} \quad (5.1.16)$$

$$\zeta_C \equiv \frac{\gamma - 1}{C_e^2} + \xi_1 \zeta_T \zeta_O + \frac{T_O}{C_{pO}} \left(\frac{\partial C_p}{\partial T} \right)_O \zeta_T^2 \quad (5.1.17)$$

$$\zeta_T \equiv \frac{(\gamma - 1) [E_1 - (\beta_T - \beta_\rho) E_3] - \gamma \beta_\rho Q}{E_1 + (\beta_T - \beta_\rho) (Q - E_3)} \quad (5.1.17)$$

$$\zeta_O \equiv \frac{(\gamma - 1) \beta_T - \beta_\rho}{E_1 + (\beta_T - \beta_\rho) (Q - E_3)} \quad (5.1.18)$$

The first two terms of order ϵ in (5.1.13) are nonlinear.

The third term, $\zeta_O^* \phi_{\tau\tau\tau}$, is linear and is actually contained

in (5.1.3). We note when the chemical reactions are ignored that $C_e = 1$, $\zeta_o^* = 0$, and $\zeta^* = \gamma - 1$, and hence (5.1.13) in this limit is easily obtained from classical inviscid second-order potential theory.

We now observe that the first-order corrections to the linear inviscid terms amount to the linear combination of the first-order linear viscous correction and the first-order nonlinear inviscid correction. Thus the full first-order correction to the potential equation is

$$\left[C_e^{2\gamma} \nabla^2 \phi - \phi_{\tau\tau} \right]_{\tau} = \epsilon \left[\frac{1}{A_4} \left(A_5 \nabla^4 \phi - B_5 \nabla^2 \phi_{\tau\tau} + P_r S_c^2 \phi_{\tau\tau\tau\tau} \right) + \frac{\partial}{\partial \tau} (\nabla \phi)^2 + \zeta^* \frac{\partial}{\partial \tau} (\phi_{\tau} \nabla^2 \phi) \right] + O(\epsilon^2) \quad (5.1.20)$$

This equation can be reduced further if we realize that to lowest order $C_e^{2\gamma} \nabla^2 \phi = \phi_{\tau\tau}$. Replacing the linear space derivatives on the right-hand side with the equivalent time derivatives then yields, correct to order ϵ ,

$$C_e^{2\gamma} \nabla^2 \phi - \phi_{\tau\tau} = \epsilon \left[\frac{A_5 - B_5 C_e^2 + P_r S_c^2 C_e^4}{A_4 C_e^4} \phi_{\tau\tau\tau\tau} + \frac{\partial}{\partial \tau} (\nabla \phi)^2 + \zeta^* \phi_{\tau} \nabla^2 \phi \right] + O(\epsilon^2) \quad (5.1.21)$$

where we have integrated once with respect to τ and set the function of integration equal to zero. Equation (5.1.21) governs the long-time behavior near the shock fronts.

The origin of the diffusion terms, that is, the coefficient of $\phi_{\tau\tau\tau\tau}$, can now be traced back to the original

linearized equation (2.3.18). Further, this same coefficient appeared in the long-time solution by Laplace transforms. In fact, we can identify the parameter b_e from equation (2.4.8) as

$$b_e \equiv \frac{1}{\sqrt{2}} \left[\frac{B_5 C_e^2 - A_5 - P_r S^2 C_e^4}{A_4 C_e^4} \right]^{-1/2} \quad (5.1.22)$$

Further insight into the nature of the nonlinear interaction can be obtained by specializing equation (5.1.21) to one-dimensional motion. If we consider an initial-value problem with boundary conditions given at $x = 0$, such as for the motion of a piston, then it is appropriate to introduce new independent variables defined as

$$\begin{aligned} \xi &= \tilde{x} - C_e \tilde{\tau} \\ X &= \epsilon \tilde{x} \end{aligned} \quad (5.1.23)$$

One would be led to such a transformation from the method of multiple scales since a straightforward perturbation expansion for equation (5.1.21) would lead to a secular nonuniformity when $\tilde{x} = O(\epsilon^{-1})$. In the new variables (5.1.23), equation (5.1.21) becomes to lowest order

$$\phi_{X\xi} + \frac{2+\zeta^*}{2C_e} \phi_\xi \phi_{\xi\xi} = \frac{B_5 C_e^2 - A_5 - P_r S^2 C_e^4}{2A_4 C_e^3} \phi_{\xi\xi\xi} + O(\epsilon) \quad (5.1.24)$$

In the new variables, ϕ_ξ is the lowest-order velocity contribution, that is,

$$v = \epsilon U + O(\epsilon^2) \quad (5.1.25)$$

where $U = \phi_{\xi}$. We can place equation (5.1.24) in a conventional form if we replace X by the new variable

$$\eta \equiv \frac{2+\zeta^*}{2C_e} X = \frac{2+\zeta^*}{2C_e} \epsilon \tilde{x} \quad (5.1.26)$$

and introduce the effective diffusivity

$$v^* \equiv \frac{B_5 C_e^2 - A_5 - P_r S_c^2 C_e^4}{A_4 C_e^2 (2+\zeta^*)} = \frac{1}{2b_e^2 (2+\zeta^*)} \quad (5.1.27)$$

Then equation (5.1.24) becomes for the velocity $U(\xi, \eta)$

$$U_{\eta} + UU_{\xi} = v^* U_{\xi\xi} + O(\epsilon) \quad (5.1.28)$$

We recognize this nonlinear diffusion equation as the famous Burgers' equation. Burgers' equation can be solved exactly [30,44,45]. Distinct solutions of this equation have been tabulated in a paper by Benton and Platzman [46]. To lowest order, the other perturbation variables are found to be

$$\begin{aligned} p' &= \epsilon \gamma C_e U + O(\epsilon^2) \\ \rho' &= \frac{\epsilon}{C_e} U + O(\epsilon^2) \\ T' &= \epsilon \zeta_T C_e U + O(\epsilon^2) \end{aligned} \quad (5.1.29)$$

$$Y'_F / fW_F = Y'_X / \chi W_X = -\epsilon \zeta_O C_e U + O(\epsilon^2)$$

Note that the effective diffusivity v^* is related to the parameter b_e in the linear theory, equation (5.1.22), by the relation $2(2+\zeta^*)b_e^2 v^* = 1$, where ζ^* has something to do with the second derivatives of rate of reaction function R .

Thus linear theory yields the correct combination of terms arising from viscous, thermal, mass-diffusion, and chemical reaction dissipation that contribute to the breadth of the shock front, but raised to the wrong power.

CHAPTER VI

CONCLUDING REMARKS

In this investigation, a ternary gas mixture initially in chemical equilibrium, or nearly so, has been considered. A small temperature or pressure perturbation disturbs the gas mixture, and the subsequent responding gas motion has been determined for small disturbances. In particular, the problems of hot-surface ignition and the one-dimensional weak-explosion problems have been studied. The results illustrate the combined effects of viscosity, thermal conduction, mass diffusion, and chemical nonequilibrium on the propagation of small disturbances in reacting gas mixtures. The embryonic structures of both detonation and deflagration waves are obtained as natural outputs of the analysis. The results are of a fundamental theoretical interest that contribute to the basic knowledge and understanding of transient combustion and chemical-reaction problems. They are also of some practical utility, especially with regards to the propagation of acoustic disturbances.

The attack on the problem was by means of linearized theory. By this method, a general methodology and approxi-

mation scheme was established that applies to a wide class of problems. As in most linearized approximations, the results break down in certain limiting regimes. In this regard the nonlinear evolution of the weak detonation wave front was analyzed and found to be governed by Burgers equation for one-dimensional problems. The effects of viscosity, thermal conduction, mass diffusion, and chemical reactions on the effective diffusivity were established.

The present theory can also be applied to other exemplary problems, such as the piston problem, the cylindrical and spherical explosion problems, the hot-spot problem, the hot-surface ignition problem including surface catalycity, and the spark-ignition problem. The study of these problems would be both interesting and useful. Also the effects of pressure-diffusion and thermo-diffusion on the resulting gas motion, or other dissipative effects such as radiation or electric and magnetic fields might be studied fruitfully by this approach.

REFERENCES

1. Friedman, R. and Burke, E., "A Theoretical Model of a Gaseous Combustion Wave Governed by a First-Order Reaction", Journal of Chemical Physics, Vol. 21, No. 4, 710-714 (1953).
2. Spalding, D.B., Stephenson, P.L., and Taylor, R.G., "A Calculation Procedure for the Prediction of Laminar Flame Speeds", Combustion and Flame, 17, 55-64 (1971).
3. Bledjian, L., "Computation of Time-Dependent Laminar Flame Structure", Combustion and Flame, 20, 5-17 (1973).
4. Vance, G.M. and Krier, H., "A Theory for Spherical and Cylindrical Laminar Premixed Flames", Combustion and Flame, 22, 365-375 (1974).
5. Smoot, L.D., Hecker, W.C. and Williams, G.A., "Prediction of Propagating Methane-Air Flames", Combustion and Flame, 26, 323-342 (1976).
6. Williams, F.A., "Theory of Combustion in Laminar Flows", Annual Review of Fluid Mechanics, Vol. 3, 171-188 (1971).
7. Bush, W.B. and Fendell, F.E., "Asymptotic Analysis of Laminar Flame Propagation for General Lewis Numbers", Combustion Science and Technology, Vol. 1, 421-428 (1970).
8. Berman, V.S. and Riazantsev, I.S., "Analysis of the Problem of Thermal Flame Propagation by the Method of Matched Asymptotic Expansions", PMM, Vol. 36, No. 4, 659-666 (1972).
9. Clarke, J.F., "The Pre-mixed Flame with Large Activation Energy and Variable Mixture Strength: Elementary Asymptotic Analysis", Combustion Science and Technology, Vol. 10, 189-194 (1975).

10. Williams, F.A., "Quasi-steady Gas-phase Flame Theory in Unsteady Burning of a Homogeneous Solid Propellant", AIAA J., 11, 1328-1330 (1973).
11. Ludford, G.S.S., "Combustion for Large Activation Energy", Letters in Applied and Engineering Sciences, Vol. 4, 49-62 (1976).
12. Buckmaster, J.D., Kapila, A.K., and Ludford, G.S.S., "Linear Solid Deflagration for Large Activation Energy", Acta Astronautica, Vol. 3, 593-614 (1976).
13. Clarke, J.F., "Parameter Perturbations in Flame Theory", Prog. Aerospace Science, Vol. 16, No. 1, 3-29 (1975).
14. Clarke, J.F., "The Laminar Diffusion Flame in Oseen Flow: The Stoichiometric Burke-Schumann Flame and Frozen Flow", Proc. Roy. Soc. A 296, 519-545 (1967).
15. Clarke, J.F., "The Laminar Diffusion Flame Behind a Blunt Body: A Constant-Pressure Oseen-Flow Model", J. Inst. Maths. Applics., 3, 347-361 (1967).
16. Rasmussen, M.L., "Diffusion Flames Associated with Weak Explosions", Aero Note 2-74, Cranfield Institute of Technology, Aerodynamics Division, Cranfield, Bedford, England (1974).
17. Rasmussen, M.L., "Acoustic Motion Induced by a Diffusion Flame", AIAA Paper No. 75-525. Presented at 2nd AIAA Aero-Acoustics Conference, Hampton, Virginia, March 24-26. Also in Aeroacoustics: Jet Noise, Combustion, and Core Engine Noise, Vol. 43, Progress in Astronautics and Aeronautics, MIT Press, 531-554 (1976).
18. Rasmussen, M.L., "Acoustic Disturbances Produced by an Unsteady Spherical Diffusion Flame", Proceedings of the 13th Annual Meeting, Society of Engineering Science, Advances in Engineering Science, Vol. 4, NASA CP-2001, 1653-1664 (1976).
19. Williams, F.A., "Linearized Analysis of Constant-Property Duct Flows", J. of Fluid Mechanics, Vol. 34, Part 2, 241-261 (1968).
20. Moore, F.K. and Curtis, J.T., "Weak, Nonequilibrium, Diffusive Waves in a Dissociated Gas", Proceedings of the 1960 Heat Transfer and Fluid Mechanics Institute, Stanford University Press, 164-175 (1960).

21. Sforza, P.M. and Bloom, M.H., "Linearized Analysis of Diffusing, Relaxing Gas Flow", Physics of Fluids, Vol. 8, No. 1, 36-43 (1965).
22. Rasmussen, M.L., "Large Time Inversion of Certain Laplace Transforms in Dissipative Wave Propagation", Journal of Engineering Mathematics, Vol. 9, No. 3, 261-265 (1975).
23. Hirshfelder, J.O., Curtis, C.F., and Bird, R.B., Molecular Theory of Gases and Liquids. John Wiley and Sons, New York (1954).
24. Zhdanov, V.M. and Skachkov, P.P., "Transport Equations for Chemical Reactions in an Inhomogeneous Gas Phase", Fluid Dynamics, Vol. 7, No. 3, 473-483 (1972).
25. Clarke, J.F. and McChesney, M., The Dynamics of Real Gases. Butterworths, London (1964).
26. Vincenti, W. and Kruger, C., Introduction to Physical Gas Dynamics, Wiley, New York, 467-469 (1965).
27. Wu, T. Yao-Tau, "Small Perturbations in the Unsteady Flow of a Compressible, Viscous, and Heat-Conducting Fluid", J. Math. and Phys. 35, No. 1, 13-27 (1956).
28. Lick, W., "Wave Propagation in Real Gases", in Advances in Applied Mechanics, G. Kuerti, editor, Vol. 10, Academic Press, New York (1967).
29. Whitham, G.B., "Some Comments on Wave Propagation and Shock-Wave Structure with Application of Magneto-hydrodynamics", Communications in Pure and Applied Math., Vol. 12, 113-158 (1959).
30. Whitham, G.B., Linear and Nonlinear Waves, John Wiley and Sons, New York (1974).
31. Hirschfelder, J.O., Curtiss, C.F. and Campbell, D.E., J. Phys. Chem., 57, p. 403 (1953).
32. Williams, F.A., Combustion Theory, Addison-Wesley, Reading, Mass. (1965).
33. Merzhanov, A.G. and Averson, A.E., "The Present State of the Thermal Ignition Theory: An Invited Review", Combustion and Flame, 16, 89-124 (1971).

34. Kim, S.C. and Chung, P.M., "An Asymptotic, Thermo-Diffusive Ignition Theory of Porous Solid Fuels", Journal of Heat Transfer, Vol. 98, No. 2, 269-275 (1976).
35. Shkadinskii, K.G. and Barzykin, V.V., "Hot-Surface Ignition of Gases with Allowance for Diffusion and Hydrodynamics", Fizika goreniya i vzryva (Combustion, Explosion, and Shock Waves), Vol. 4, No. 2 (1968).
36. Merzhanov, A.G., Khaikin, B.I. and Shkadinskii, K.G., "Establishment of Steady Flame Propagation when Igniting a Gas by a Heated Surface, Zh. Prikl. Mekhan. i Tekh. Fiz. (Journal of Applied Mechanics and Technical Physics), No. 5 (1969).
37. Vilyunov, V.N., "Theory of Spark Ignition", Soviet Physics-Doklady, Vol. 18, No. 1, 40-42 (1973).
38. Carslaw, H.S. and Jaeger, J.C., Operational Methods in Applied Mathematics, Dover, New York (1963).
39. Averson, A.E., Barzykin, V.V. and Merzhanov, A.G., "Laws of Ignition of Condensed Explosive Systems with Perfect Heat Transfer at the Surface with Account for Burnup", Inzh-fiz. zh. (Journal of Engineering Physics), Vol. 9, No. 2 (1965).
40. Moran, J.P. and Shen, S.F., "On the Formation of Weak Plane Shock Waves by Impulsive Motion of a Piston", J. Fluid Mech., Vol. 25, Part 4, 705-718 (1966).
41. Halabisky, L. and Sirovich, L., "Evaluation of Finite Disturbances in Dissipative Gasdynamics", Physics of Fluids, Vol. 16, No. 3, 360-368 (1973).
42. Rasmussen, M.L., "Evolution of Weak Disturbances in Inert Binary Mixtures", Dept. of Aeronautics and Astronautics, Stanford University, Joint Institute for Aeronautics and Acoustics Report JIAA TR-6 (1977).
43. Rasmussen, M.L. and Frair, K.L., "Diffusion Effects on Weak Spherical Disturbances in Binary Mixtures", Developments in Theoretical and Applied Mechanics, Vol. 8, 589-601 (1976).
44. Cole, J.D., "On a Quasi-Linear Parabolic Equation Occurring in Aerodynamics", Quart. Appl. Math. 9, 225-236 (1951).

45. Hopf, E., "The Partial Differential Equation $U_t + UU_x = \mu U_{xx}$ ", Comm. Pure Appl. Math. 3, 201-230 (1950).
46. Benton, E.R. and Platzmann, G.W., "A Table of Solutions of the One-Dimensional Burgers' Equation", Quart. Appl. Math., 30, 195-212 (1972).
47. Erdelyi, A., Asymptotic Expansions, Dover, New York (1956).

APPENDIX A

SEVENTH-ORDER PARTIAL DIFFERENTIAL EQUATION FOR THE VELOCITY POTENTIAL

If Fick's law of diffusion is assumed in the very beginning of formulation, the analysis could be less complicated. The problem is then governed by the following set of linearized equations:

Continuity

$$\rho_{\tau} = -\nabla^2 \phi \quad (\text{A.1})$$

Momentum

$$P = \gamma (\nabla^2 \phi - \phi_{\tau}) \quad (\text{A.2})$$

Species

$$D_S Y_X = -S_C \chi W_X \tilde{R} \quad (\text{A.3})$$

$$D_S Y_F = -S_C f W_F \tilde{R} \quad (\text{A.4})$$

Energy

$$D_P T = \frac{\gamma-1}{\gamma} P_{\tau} P_{\tau} + P_{\tau} Q \tilde{R} \quad (\text{A.5})$$

State

$$P = \rho + T + \alpha_X Y_X + \alpha_F Y_F \quad (\text{A.6})$$

The linearized rate of reaction function, \tilde{R} , is given by

equation (2.3.4). The above equations can be manipulated so that the following single seventh-order equation for ϕ is obtained:

$$\begin{aligned} & \gamma \nabla^6 \phi_{\tau} + \nabla^4 \left[\nabla^2 \phi - \alpha \phi_{\tau\tau} \right] + \nabla^2 \left[\beta_1 \phi_{\tau\tau} - \beta_2 \nabla^2 \phi \right]_{\tau} + P_r S_c \left[\nabla^2 \phi - \phi_{\tau\tau} \right]_{\tau\tau} \\ & \nabla^2 \left[\beta_3 \phi_{\tau\tau} - \beta_4 \nabla^2 \phi \right] + P_r S_c \left[E_1 + (\beta_T - \beta_{\rho}) (Q - E_3) \right] \left[\nabla^2 \phi - \frac{1}{C_e^2} \phi_{\tau\tau} \right]_{\tau} \\ & = S_c (\alpha_F E_1 - A_F E_3) D_P J \end{aligned} \quad (A.7)$$

where

$$\begin{aligned} \alpha & \equiv \gamma (S_c + 1) + P_r \\ \beta_1 & = S_c (\gamma + P_r) + P_r \\ \beta_2 & = P_r + S_c (1 + \gamma E_1) + \gamma \beta_T (P_r Q - S_c E_3) \\ \beta_3 & = S_c E_1 (\gamma + P_r) + \gamma \beta_T \left[P_r Q (S_c + 1) - S_c E_3 (P_r + 1) \right] \\ \beta_4 & = S_c E_1 + (\beta_T - \beta_{\rho}) (P_r Q - S_c E_3) \end{aligned} \quad (A.8)$$

where the variable $J(x, \tau)$ is defined as

$$J(x, \tau) = Y_F - \sigma Y_X \quad (A.9)$$

and satisfies the diffusion equation, that is $D_S J = 0$. The notation σ is the stoichiometric mass ratio, namely $\sigma \equiv f W_F / \chi W_X$. For the case of hot-surface ignition of gases, it is found that $J(x, \tau) = 0$ identically.

A similar equation has been developed and studied by Rasmussen and Frair [43] and Rasmussen [42] for inert

binary mixtures. The present analysis extends those investigations to include chemical reactions. The last two terms in the left hand side of equation (A.7) reflect the effect of chemical reaction. Also the coefficients have been modified.