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THE STEADY-STATE THEORY OF IGNITION OF FLOWING GASEOUS MIXTURES BY HOT SURFACES

A THESIS

Presented to

The Faculty of the Division of Graduate

Studies and Research

by

Alexandros Costas Alkidas

In Partial Fulfillment

of the Requirements for the Degree

Doctor of Philosophy

In the School of Mechanical Engineering

Georgia Institute of Technology

March, 1972

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THE STEADY-STATE THEORY OF IGNITION OF FLOWING

GASEOUS MIXTURES BY HOT SURFACES

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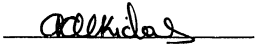

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SUMMARY

The primary objective of this work was to investigate the ignition of a combustible gaseous mixture by a heated surface, employing a steady-state analytical approach. A general equation based on similarity analysis was developed that expresses the surface temperature of the body in terms of heat, mass, and chemical parameters of the flow.

Using the stagnation region of an axisymmetric blunt body as a working example, the ignition characteristics of the above flow were obtained by examining the surface heat transfer-First Damköhler number relationship. From this plot two critical parameters were obtained: the Ignition First Damköhler number $\bar{D}_{I,i}$ and the Extinction First Damköhler number $\bar{D}_{I,e}$. The transition from frozen to equilibrium state (Ignition) occurs at $\bar{D}_I = \bar{D}_{I,i}$. Likewise, the transition from equilibrium to frozen state (Extinction) occurs at $\bar{D}_I = \bar{D}_{I,e}$.

Using the same working example the ignition of the gaseous mixture was examined by means of the Van't Hoff's criterion. This condition can be mathematically expressed as $\partial T/\partial \hat{n} = 0$. A comparison of the two methods showed close agreement.

Finally, an expression of the Ignition First Damköhler number in terms of the surface temperature of the heated body was obtained using a simplified model of the heat interactions in the gas-solid interface.

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NOMENCLATURE

Symbol

English Letters

a	coefficient of the potential flow velocity
A	pre-exponential constant (explosion theory)
B	overall frequency factor
B	$Eq^{o}w_{o}/pc_{v}RT_{o}^{2}$ (explosion theory)
C	$\rho\mu/\rho_{e}\mu_{e}$
c_{p}	specific heat at constant pressure
c_{v}	specific heat at constant volume
d	diameter of jet
$\vec{d}_{j}$	defined by Equation (4)
D	mass diffusivity
D_{ij}	binary mass diffusivity for species pair i-j
$D_{T,i}$	thermal diffusivity for species i
D_{I}	the Damköhler's First dimensionless group, $w_{o}L/\rho u_{o}$
D_{II}	the Damköhler's Second dimensionless group, $q^{o}/c_{p,o}T_{o}$
D_{III}	the Damköhler's Third dimensionless group, $D_{I}\cdot D_{II}$
$\bar{D}_{I}$	$\frac{1}{2}\gamma_{O}W_{O}Y_{F,e}(B\rho_{e}/a)$
$\bar{D}_{I,e}$	Extinction First Damköhler number
$\bar{D}_{I,i}$	Ignition First Damköhler number
$\bar{D}_{II}$	$q^{o}Y_{F,e}/c_{p,e}T_{e}\gamma_{F}W_{F}$
E	activation energy
E^{*}	E/RT_{e}, dimensionless activation energy

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English Letters (Continued)

Ec	Eckert number, $u_o^2/c_{p,o}T_o$
f'	u/u_e, dimensionless velocity
f_i	force per unit mass of species i
Fr	Froude number, u_o^2/gL
h	specific enthalpy
h_i^o	standard heat of formation per unit mass of species i
$\underline{I}$	unit tensor
k	thermal conductivity
k_b	backward reaction rate constant
K_c	equilibrium constant
k_f	forward reaction rate constant
Le	Lewis number
n	number of moles per unit volume
n	order of the chemical reaction (explosion theory)
$\hat{n}$	unit surface vector
N	total number of chemical species present
n_e	dimensionless "stoichiometry," Equation (52)
n_i	molar concentration of species i
Nu	Nusselt number, $q_w x/k(T_e-T_w)$
p	hydrostatic pressure
Pr	Prandtl number, $c_{p,o}\mu_o/k_o$
$\vec{q}$	heat flux vector
q^o	standard heat of reaction
q_{ch}	surface heat transfer due to chemical reaction

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English Letters (Continued)

q_{con}	convective heat transfer
q_{gen}	heat generated by chemical reaction
q_{lost}	heat lost to the surroundings
R	universal gas constant
R_D	$\bar{D}_I/\bar{D}_{II}$
r_o	cylindrical radius of surface
r_o	principal dimension of the vessel (explosion theory)
Re	Reynolds number, $\rho_o u_o L/\mu_o$
s	$\int_0^x \rho_e \mu_e u_e r_o^2 dx$
Sc	Schmidt number, $\mu_o/\rho_o D_o$
t	time
t_r	residence time
T	temperature
T^o	standard reference temperature
T_o	temperature of the heated wall (explosion theory)
u	specific internal energy
u	component of velocity in x-direction
v	component of velocity in y-direction
$\vec{v}$	macroscopic velocity vector
$\vec{V}_i$	diffusion velocity vector of species i
w_i	rate of production of species i by chemical reaction
W	molecular weight of the mixture
W_i	molecular weight of species i
w_o	initial concentration of the reactants (explosion theory)

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English Letters (Continued)

x	distance along surface
X_i	mole fraction of species i
y	distance normal to surface
Y_i	mass fraction of species i

Greek Letters

α_i	$Y_i/Y_{i,e}$
β	defined by Equation (61)
δ	boundary layer thickness
δ	ignition parameter (explosion theory)
ϵ	RT_o/E (explosion theory)
η	$[(\rho_e u_e r_o)/(2s)^{1/2}]\int_0^y (\rho/\rho_e)dy$
θ	T/T_e, dimensionless temperature
Θ	$E(T-T_o)/RT_o^2$ (explosion theory)
θ_m	maximum wall temperature, Equation (91)
κ	bulk viscosity
μ	viscosity
M_i	chemical designation of species i
γ	kinematic viscosity
γ_i	stoichiometric coefficient of the ith species
$\underline{\pi}$	pressure tensor
ρ	density
$\underline{\tau}$	viscous stress tensor
$\underline{\tau}^D$	diffusion stress tensor
ψ	stream function, Equation (41)

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Subscripts

e	free stream
F	fuel
i	ith species
N	inert gas
O	oxidant
o	a reference state
P	products
w	at the wall surface

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CHAPTER I

INTRODUCTION

The ignition of gaseous mixtures is considered one of the most typical but important phenomena in the field of combustion. It is the process by which a propagating flame is originated in the mixture. Its importance was recognized quite early and analytical and experimental work was undertaken by the combustion researchers in order to shed some light on its complex mechanisms and the factors affecting them. Various methods have been used by which combustible gaseous mixtures have been ignited. These methods are:

a. Heated surfaces

b. Pilot flames

c. Hot gases

d. Shock waves

e. Capacitance sparks

f. Inductance sparks

In the past two decades, due to the development of high speed air vehicles, the study of ignition in forced convection systems grew to be of considerable importance. Ignition in the combustor of such a vehicle can be attained by any of the above-listed methods. However, ignition by electrical discharge appears to be the most efficient method. Ignition by shock waves is impractical and pilot flames or hot gases require an additional ignition source to produce the pilot flame or hot gases in

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the first place. An additional disadvantage of the two latter methods is that due to their low energy interchange with the flowing mixture and the short resident time available (high speed stream), a larger combustor is required. Compared to spark ignitors, heated surfaces have a much longer response time, making them inefficient ignitors. The long response time can be attributed to the external heat source needed to raise the temperature of the surface to the required value. However, an aspect of heated surfaces that is worth considering as an ignition source of high speed flow is their dual role as an ignition source and a flameholder. A high velocity combustible mixture will ignite and stabilize near the surface of a heated body where the flow velocity is less or equal to the flame velocity of the mixture. Thus, a continuous ignition source for the incoming fresh mixture is formed.

Another typical application of ignition by hot surfaces is the ignition of a combustible mixture by a hot projectile travelling at a moderate speed. In such a problem, the minimum surface temperature of the projectile necessary to ignite the combustible mixture, is required. This temperature is a function of the speed of the projectile.

The study considered here pertains to the case of ignition of a flowing gaseous mixture by a hot surface. A complete study of this problem involves the investigation of the effects of temperature, velocity, and the chemical parameters (type of fuel and oxidizer) of the combustible mixture, on the wall temperature of the body (ignition temperature).

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The very early investigations on ignition by hot surfaces dealt with static mixtures, i.e., explosive mixtures in a container with heated walls. The analytical theories developed were called thermal explosion theories because of the omission of the diffusion processes. They investigated the relation between the heat generated by a chemical reaction, and the heat lost to the surroundings, primarily by conduction. These theories explored the critical limits beyond which the stationary solution of the governing equations became impossible. The existence of the critical conditions is assured by the fact that the heat generated by chemical reaction is approximately exponential while the heat lost to the surroundings is approximately linear with respect to the temperature. The problem for the establishment of the critical conditions was reduced to the determination of a critical dimensionless parameter δ_{cr}. This parameter is a function of the wall temperature, vessel size, physical and chemical properties of the mixture. For $\delta > \delta_{cr}$ the reactive mixture will be ignited while for $\delta < \delta_{cr}$ the mixture will be heated until it reaches a steady-state.

Some of the early investigators in the field of ignition of a forced convection system by a hot surface, immersed a heated body such as a wire or a cylinder in a stream of combustible mixture. Ignition was initiated in the wake of the body where the velocity was low. Unfortunately, due to the complexity of the flow patterns the interpretation of the experimental results by analytical methods was not very successful. Subsequent studies of ignition were made in the laminar boundary layer of a plane surface or in the stagnation region of a blunt

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body where the flow patterns are much simpler. From these studies the length of the hot surfaces required for the stabilization of the flame was determined. In the case of stagnation flow the surface temperature of the body required to ignite the combustible mixture was obtained.

As an ignition criterion in reactive flows, the Van't Hoff's critical condition for ignition was used. This condition states that a combustible mixture near the non-catalytic surface of a hot body will ignite when the temperature gradient normal to the wall is zero. It is a limiting condition. It implies that ignition will occur when the heat lost to the surroundings by conduction and convection is equal to the heat generated by the chemical reaction. The physical meaning of the above condition can be understood by considering the heat transfer processes resulting when a stream of reactive mixture comes in contact with a hot surface. Due to the higher temperature of the wall, heat will be transferred to the gas, resulting in an increase of the gas temperature. This temperature rise will bring about an increase in the self-heating of the gas, where the heat release by a chemical reaction is inversely proportional to the exponential of the temperature. The heat generated in turn will further raise the temperature of the gas, thus reducing the net heat flux through the wall. Hence the adiabatic condition of the wall is an indication that the temperature of the mixture has risen sufficiently to sustain chemical reaction.

As has been stated in the above discussion, Van't Hoff's ignition criterion is an indication of the self-heating processes occurring in the mixture and it is not a sufficient condition of ignition. In the case

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of ignition of a static mixture in an unsymmetrical heated vessel, the Van't Hoff's criterion is only a good approximation. However, it has been applied in the studies of ignition of forced convection systems by heated surfaces. As yet, there is no proper mathematical proof of its validity.

It is well established that the phenomenon of ignition of a reactive gaseous mixture by a hot surface is governed by the heat interactions occurring in such a system. In general, ignition can be considered as the transient process by which the state of the system changes from "frozen" to "equilibrium." Such a change affects the value of the surface heat transfer, which is altered from a minimum for frozen flow to a maximum for equilibrium flow. Thus it is apparent that an examination of the influence of the degree of reactivity of a combustible mixture on the surface heat transfer is required.

Similarity considerations in the field of combustion reveal the existence of two dimensionless groups in addition to the well-known dimensionless parameters obtained for non-reactive mixtures. These two parameters, the First Damköhler number, D_I, and the Second Damköhler number, D_{II}, are characteristic of the chemical processes in the flow field. The parameter D_I represents the ratio of the convective time to the chemical time, while the parameter D_{II} represents the ratio of the heat addition by chemical reaction to the heat addition associated with the convection of enthalpy.

In chemically reacting flows the transition between the two limiting states, namely frozen and equilibrium flow, can be described by the

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First Damköhler number. For $D_I >> 1$ the chemical reaction time is much shorter than the residence time of the gas particles, and the system is regarded as existing in thermodynamic equilibrium. On the other hand, for $D_I << 1$ the convection time is much shorter than the chemical time; the gas particles do not have time to react, and the state of the system is essentially frozen. As stated above the degree of reactivity of chemically reacting flows past solid boundaries is directly related to the surface heat transfer rates to and from the boundaries. Consequently, the problem is reduced to a study of the effect of the First Damköhler number on the surface heat transfer rate.

The present work on the ignition characteristics of a flowing combustible mixture by a hot surface has been carried out with the following objectives in mind:

1. Demonstrate the importance of the First Damköhler Similarity parameter on the ignition studies of forced convection systems in contact with hot surfaces.

2. Investigate the validity of Van't Hoff's ignition criterion in the case of ignition of flowing combustible mixtures.

3. Study the effects of the velocity, temperature, and concentration of inert gases of the mixture on the ignition temperature. Also included in this objective are the value of the chemical kinetics and the effects of the activation energy on the ignition temperature.

4. Develop and test a highly simplified theory analogous to the present approximate thermal theories.

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The first objective consists of investigating the influence of the First Damköhler number D_I on the surface heat transfer of a combustible mixture past a solid boundary at a given constant temperature. The effect of this parameter on the surface heat transfer can be obtained by solving the steady-state form of the equations describing the reacting flow for a range of values of the parameter D_I corresponding to the transition from frozen to equilibrium flow. It must be noted that the differential equations governing the flow are highly non-linear because of the exponential reaction rate term. This mathematical difficulty excludes any possible analytical approach and can be resolved only through the use of numerical analysis. Any attempt to linearize the governing equations (the usual procedure in fluid dynamics) will prove disastrous, since the critical conditions are dependent on the non-linear nature of the problem. A plot of the surface heat transfer versus the First Damköhler Similarity parameter will indicate the transition from frozen (minimum surface heat flux) to the equilibrium state (maximum surface heat flux) of the equations. One may anticipate that such a plot will be useful in studying the ignition characteristics of forced convection systems. A plot of the value of the reactant mass fraction at the wall versus the First Damköhler number will serve this purpose equally well, since the two limiting chemical states of the mixture, i.e., frozen and equilibrium, can be identified by the value of the reactant mass fraction at the wall.

It is apparent from the above discussion that the ignition characteristics of a flowing reactive mixture can be examined with

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consideration only of the steady-state solution of the conservation equations. This is in contrast to the nature of the ignition process, which is basically a transient one. The disadvantage of this method is its inability to predict the ignition lag (defined as the time between the introduction of the mixture to the ignition source, in this case a heated surface, and the first indication of ignition). The ignition lag or the ignition time as it is most commonly referred to, is of prime importance in the design of combustion chambers, since it can affect the combustion efficiency of a combustor.

In order to evaluate the Van't Hoff ignition criterion, the flow configuration and flow properties (free stream temperature, physical properties, and type of fuel and oxidizer) used in Objective 1, will be utilized to determine the ignition temperature (wall temperature). The ignition temperature will be treated as an eigenvalue by introducing the critical ignition condition $\partial T/\partial \hat{n} = 0$ as an additional boundary condition of the differential equations governing the reactive flow.

The parameter D_I is a measure of the convective time relative to the chemical time; consequently, a correlation between the First Damköhler number and the ignition temperature will show: a) the influence of the free stream velocity of the mixture on the ignition temperature, T_w, when the chemical time is kept constant (i.e., the same type of fuel and oxidizer) and b) the influence of the chemical kinetics on the ignition temperature with constant free stream velocities.

Finally, a simplified theory will be developed using the concept of a reduced film of quiescent gaseous mixture close to the surface of

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the heated body. This model can be tested against the numerical results.

The analysis reported here will be restricted to the study of the ignition characteristics of a cold combustible mixture at the forward stagnation point of a non-catalytic blunt body. The surface temperature of the body, T_w, is assumed to be constant and at a higher value than the temperature of the incoming gaseous stream, T_e. The kinetics of the combustible mixture will be assumed to be adequately represented by one-step second-order chemical reaction.

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CHAPTER II

LITERATURE REVIEW

A. Introduction

This chapter deals with past investigations pertinent to the present problem. Past literature on ignition of combustible gases will be reviewed in three parts. Section B of this chapter examines the ignition of static mixtures and especially the two approximate theories of thermal explosion by Semenov and Frank-Kameneskii. In Section C, the ignition of flowing gas mixtures by hot surfaces is reviewed. This section is divided into two segments: Segment one deals with heated spheres and rods, and segment two with heated flat plates and blunt bodies.

Although the combustion problem considered in this study is of the premixed category, valuable information was derived from the studies of ignition and extinction of the diffusion flames. In Section D, the role of the First Damköhler Similarity parameter in the studies of ignition and extinction of initially unmixed gases, is reviewed.

B. Ignition of Static Mixtures

There are two approximate theories of thermal explosion that deal with the ignition of static mixtures enclosed in heated containers. These theories are: the steady-state theory of Frank-Kameneskii and the non-steady-state theory of Semenov. An excellent introduction to the two theories is found in the English translation of the Russian

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monographs of Semenov [1]*, Frank-Kameneskii [2], Khitrin [3], and Vulis [4].

Frank-Kameneskii [2] examined the steady-state form of the heat conduction equation with a reaction source term. Utilizing a dimensionless reaction rate parameter δ he obtained the condition $\delta = \delta_{cr}$ by which for $\delta > \delta_{cr}$ steady-state solution of the above-mentioned heat conduction equation is impossible. The parameter δ is defined by

$$\delta = (q^{o}Er_{o}^{2}/kRT_{o}^{2})Aw_{o}^{n}\exp[-E/RT_{o}]$$

where q^{o} is the heat of combustion, E is the activation energy, A is the pre-exponential constant, T_{o} is the temperature of the heated wall, w_{o} is the initial concentration of the reactants, n is the order of the chemical reaction and r_{o} is the principal dimension of the vessel. *Ignition*, or as it is most commonly called in the case of static mixtures, *explosion*, was defined as the condition when $\delta = \delta_{cr}$. In his theoretical analysis, Frank-Kameneskii used the following approximations for the exponential part of the source term.

$$\exp[E/RT] = \exp[\theta/(1+\epsilon\theta)] \approx \exp\theta\exp[-E/RT_{o}]$$

where

$$\theta = E(T-T_{o})/RT_{o}^{2}$$

---

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and

$$\epsilon = RT_o/E$$

The above approximation is valid when the temperature of the mixture at ignition is very close to the wall temperature. Analytically, he obtained the critical value of δ and the maximum possible stable temperature rise θ_{cr} in the case of a constant temperature slab, and numerically, he evaluated the above qualities for the case of a cylinder and a sphere. Later Chambre [5] demonstrated that for the latter two cases, solutions can be obtained in terms of known tabulated functions. Parks [6] studied the effect of the Frank-Kameneskii exponential approximation (i.e., $\epsilon = 0$) on δ_{cr}. He deduced that δ_{cr} is insensitive to ϵ in the range of 0 to 0.033.

Semenov [1], the originator of the unsteady theory of thermal explosion, ignored the spatial temperature distribution of the mixture in the unsteady-state energy equation. The heat transfer process was described by the introduction of an overall heat transfer coefficient. For a zero order reaction Semenov obtained the critical conditions by means of a graphical representation. The conditions characterizing the transition from a limited temperature increase to infinite temperature increase are:

$$q_{gen} = q_{lost}$$

and

$$dq_{gen}/d\theta = dq_{lost}/d\theta$$

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where q_{gen} is the heat generated by chemical reaction, and q_{lost} is the heat lost to the surroundings. Both of the original theories neglected the reactant consumption.

The effects of reactant consumption on the critical conditions were investigated by Frank-Kameneskii [2], Thomas [7], Gray and Lee [8], using Semenov's model. The above investigators obtained similar relations between the critical values of the parameter δ, with and without reactant consumption. These relations were expressed in terms of the dimensionless adiabatic temperature rise, B, where $B = Eq^{o}w_{o}/pc_{v}RT_{o}^{2}$.

Semenov defined the critical temperature as the temperature at which the first inflection point is observed in the temperature-time curve. Most authors used Semenov's definition which is applicable in the case of zero order reactions in defining the critical temperature of the mixture in the case of appreciable reactant consumption. In 1964, Adler and Enig [9,10] demonstrated that a critical ignition temperature can be defined by considering the temperature-reactant consumption curve. They showed analytically that the critical temperature Θ_{cr} is only a function of the order of the reaction. Recently, Tyler and Wesley [11] have solved numerically the simultaneous equations of heat conduction and reactant consumption for various values of the dimensionless adiabatic temperature rise B and dimensionless activation energy ϵ. The results obtained show substantial disagreement with the zero order results of the Frank-Kameneskii model.

In general, the thermal explosion theories are used primarily as an inverse combustion problem. By means of the critical conditions, the

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unknown chemical kinetics of the substance can be found. Comparison of the observed temperature rise with θ_{cr} will give the activation energy. When the activation energy is known the critical value of δ will give the reaction rate constant. A common assumption, characteristic of these theories is the omission of the diffusion processes. In the case of gaseous mixtures such an assumption is unreasonable, since the diffusion and heat conduction are of equal importance. Thus in the prediction of the kinetics of a gaseous mixture of low activation energy (appreciable reactant consumption at ignition), diffusion of the reactants should be considered.

C. Ignition of Flowing Mixtures by Hot Surfaces

1. Heated Spheres and Rods

Silver [12] was one of the first to study experimentally the ignition of forced convection systems. By shooting small spherical quartz and platinum particles through stationary combustible mixtures, he observed that the greater the diameter of the particles, the lower the ignition temperature. The particles were introduced into the gaseous mixtures at an approximate speed of 12 ft/sec. A simplified theoretical analysis based on Semenov's thermal explosion theory was performed which qualitatively agreed with the experimental results. Using the same experimental technique, Paterson [13,14] investigated the effect of particle velocity on the ignition temperature. The particle velocity range was extended to approximately 210 ft/sec. The results indicated that:

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a. The ignition temperature is a function of the diameter and velocity of the particles. The higher the velocity the higher the ignition temperature. The influence of the diameter of the particles is similar to that observed by Silver.

b. A critical speed of the particles exists beyond which ignition does not take place. This critical speed is a function of the temperature; it increases as the temperature is increased, according to a roughly linear relation.

c. The initial temperature of the mixture does not affect the ignition temperature.

A theoretical analysis was attempted along the lines followed by Silver. The critical condition was obtained by equating the heat generated by chemical reaction to the heat lost by convection. The heat transfer coefficient was expressed in terms of the Reynolds number, thus introducing the velocity into the equations. The heat generated by the chemical reaction was evaluated by assuming that the temperature across the boundary layer thickness is approximately constant and equal to the surface temperature of the particle. The analysis showed qualitative agreement with the experimental observations (a) and (b). The theory predicted a decrease of the ignition temperature with an increase of the initial temperature of the mixture, contrary to observation (c).

The most complete experimental investigation is that by Mullen *et al.* [15], who studied the ignition of high velocity streams of combustible gases by heated cylindrical rods situated with their axis perpendicular to the direction of the flow. The range of velocities

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considered was between 50 and 500 ft/sec. The effects of the stream variables (turbulence, temperature and pressure), rod variable (diameter, size, and location of heated area, and chemical and physical nature of the surface), and the mixture variables (humidity, fuel concentration, fuel type) on the ignition phenomena, were examined. The results were reported in terms of the surface temperature of the rod and the maximum stream velocity. The conclusions that are of qualitative importance to the present study are:

a. An increase of the incoming temperature of the mixture facilitated ignition. This result is contrary to the previous experimental observations [12].

b. For a given velocity, the larger the diameter of the rod the lower the ignition temperature (surface temperature of the rod).

c. The lowest ignition temperature obtained for a given velocity was with mixtures of near stoichiometric composition.

d. Ignition temperatures increased with increasing velocities. At high-speed flows, extremely high surface temperatures were required to ignite the mixtures. High-speed motion pictures taken during the experiments indicated that the ignition process initiates near the rear stagnation point of the flow where relative low speeds exist.

Kumagai and Kimura [16] examined the ignition of gaseous streams of known turbulent intensity, by heated wires. For the range of velocities reported (0.6-90 ft/sec) the influence of turbulence of the incoming mixture on ignition was not appreciable.

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Khitrin and Goldenberg [17] attempted to correlate the results of Silver, Paterson, and Mullen *et al.*, by developing a thermal theory of ignition of flowing gas mixtures. Although more sophisticated, their approach does not differ much from that of Paterson [13]. The boundary layer surrounding the heated body was assumed to be quiescent. The Van't Hoff's criterion was used as the limiting condition for ignition. The heat transfer interaction between the wall and the mixture was described in terms of two processes: 1) heat convection expressed as a product of the temperature difference between the free stream and the wall and a heat transfer coefficient which is a function of Reynold's number; and 2) heat generated which was expressed as an integral of the rate of reaction with respect to temperature. This integral was evaluated approximately by assuming that most of the reaction occurs near the wall where the temperature is higher. For the correlation between the results, the experimental sets of data were normalised with respect to a single set, in order to eliminate the chemical kinetic constant which is unknown. From the correlations, numerical values of the activation energy were obtained.

Adomeit [18] based his theoretical investigation of the thermal ignition of flowing combustible gases on similarity concepts. He had found that in most cases the experimental results can be correlated in terms of two non-dimensional quantities, one representing the temperature of the wall and the other, the overall heat generation by the chemical reaction.

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2. Flat Plates and Blunt Bodies

Early analytical studies of combustion in flowing gaseous mixtures were confined to the plane, one-dimensional flame front. Marble and Adamson [19] were the first to consider such a problem using boundary layer approximations. They studied the ignition and combustion in the laminar mixing zone of two parallel moving gaseous streams; one stream consisted of a cool combustible mixture and the other of hot combustion products. It was argued that in the ignition region since the heat added by chemical reaction is small, the effect of combustion, on the velocity, temperature, and composition profiles obtained for the corresponding frozen flow problem can be treated as a perturbation. They postulated that ignition occurs at the point in the flow field where a "bulge" in the temperature profile is formed. Although no extinction phenomena have been obtained, it was shown that in some instances the flame detachment distance (distance between the point where the two streams meet and the point at which the temperature profile first exhibits a vertical tangent) becomes so large that it exceeds the physical dimensions of any apparatus. In their analysis first order Arrhenius kinetics were used.

The ignition of a combustible mixture in the laminar boundary layer of a constant temperature flat plate has been treated by several investigators [20,21,22]. Their aim was to obtain the distance downstream of the leading edge where ignition first occurs. This characteristic length is indicative of the minimum length of a plate required to stabilize a flame. The point at which ignition occurs was identified

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by the condition that the temperature gradient normal to the wall is zero. Along its characteristic length the plate acts as a heat source and in the remaining part as a heat sink. Dooley [20] treated the problem of thermal decomposition of azomethane. The Lewis number was assumed to be unity. In order to obtain a similarity function relating the temperature to the species mass fraction, he arbitrarily specified the chemical composition at the surface of the plate. An iterative procedure was developed to obtain an analytical solution of the energy equation. Toong [21] studied the problem of ignition by a hot flat plate, both theoretically and experimentally. He expressed the solutions of the energy and conservation of species equations in power series with respect to the non-dimensional tangential coordinates. Utilizing these series the original conservation equations were transformed to a set of non-homogeneous ordinary differential equations. Solutions were obtained numerically up to the fifth term of the series. At a certain distance along the plate, depending on its temperature, the convergence of the series became very poor. This distance was slightly longer than the computed characteristic length of the plate. Recently, the nonlinear partial differential equations describing the reactive flow over a flat surface were solved numerically by Sharma and Sirignano [22]. The reaction kinetics of the propane-air mixture were represented by a two-term, single step, second order Arrhenius expression. The first term represented the overall chemical reaction below 1250°K, while the other was above 1250°K. The effects of wall temperature, plate length, free stream velocity and Lewis number on the ignition

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point were determined. As was expected the characteristic length increased with decreasing surface temperature and increasing free stream velocity. The value of the Lewis number did not appreciably influence the location of the ignition point.

Shakhnov [23] studied the ignition and combustion of a stoichiometric mixture in the laminar supersonic boundary layer of a flat plate. The conservation equations were integrated numerically by the method of the grids. The characteristic length of the plate was defined as the tangential coordinate at which the flame front goes out of the boundary layer.

At present, only two analytical investigations have been carried out on the ignition of premixed stagnation point flows. In both cases the Van't Hoff's condition was used as an ignition criterion. Chambre [24] considered the problem of ignition of a planar stagnation flow. Utilizing certain approximations, he obtained analytical solutions of the energy equation. An ignition criterion which related the wall temperature with heat, mass, and chemical kinetic parameters was derived. His analysis was restricted to the case in which the Lewis number is unity and the dimensionless activation energy E/RT_w is very large. The chemical kinetics of the flow, in this work were described by a direct first-order reaction.

Sharma and Sirignano [25], using a second-order rate law, have numerically solved the plane and axisymmetric reactive stagnation point flows by the method of quasi-linearization. This method linearizes the equations about an assumed solution and by means of an iterative cycle

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the solution of equations converges to the non-linear solution. It must be noted that the differential equations were expressed in an implicit finite form and then solved by the "line inversion" procedure. The surface temperature of the wall (ignition temperature) was obtained for a limited range of the First Damköhler number. The effects of varying the values of the Schmidt and Prandtl transport parameters were shown to be relatively minor. For plane stagnation flow they have extended Chambre's approximate analysis to second order reaction.

D. Ignition and Extinction of Initially Unmixed Gases: The Influence of the First Damköhler Number

The assumption of infinite chemical kinetics or as it is alternatively known, the Burke-Schumann assumption [26], is often used to describe analytically, diffusion flames. Although this assumption renders an adequate model for the calculation of the flame shape and the rate of fuel consumption, its usefulness ceases to exist when the phenomena of ignition and extinction are considered, and the maximum temperature in the flame zone is required.

The above shortcomings of the model were remedied by the introduction of finite chemical kinetics [27,28,29,30], which account for the flammability limits by lowering the flame temperature.

The influence of the First Damköhler number on the ignition temperature and extinction characteristics of initially unmixed gases was first demonstrated by Fendell [31]. He considered the ignition and extinction of diffusion flames near the stagnation region, when an oxidant is blown from upstream infinity at a fuel reservoir with a

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surface perpendicular to the stagnation stream-line. A direct one-step second order reaction of the Arrhenius type was used to describe the chemical kinetics of the flow. The flow was assumed to be inviscid. The dependence of the maximum temperature (flame temperature) on the First Damköhler number was utilized to establish the ignition and extinction characteristics. For values of the Damköhler number corresponding to near-frozen and near-equilibrium conditions, asymptotic techniques established the maximum temperature dependence. For intermediate values, numerical methods were used. The flammability limits were demonstrated by the multivalued nature of the transition from frozen to equilibrium conditions. Chung, *et al.* [32] analyzed the problem of a diffusion flame in the stagnation region of a blunt body by means of boundary layer approximations. Using physical intuition they derived criteria by which the single and multiple transitions between frozen and equilibrium states are distinguished from each other.

Jain and Mucunda [33] had studied the ignition and extinction characteristics for two flow geometries: (1) a jet impinging on a wall of combustible material, and (2) the opposed jet diffusion flame. In their analysis, the effects of different approximations used for the fluid mechanics of the flow were evaluated. The ignition and extinction characteristics were obtained by plotting the First Damköhler number versus the gradient of oxidant concentration at the origin. Subsequently, it was shown that the above method was equivalent to that of Fendell's (maximum temperature versus First Damköhler number). For case one, the effects of varying the wall temperature were observed; while in

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case two, the effects of jet temperature, activation energy, and free stream oxidant concentration were investigated.

Recently Jain and Mucunda [34] have considered the extinction of an opposed jet diffusion flame with competitive reactions.

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CHAPTER III

FORMULATION OF THE PROBLEM

A. Introduction

This chapter presents the mathematical formulation of the flow of a combustible mixture at the stagnation region of an axisymmetric blunt body. The formulation is introduced in Section B with the general form of the conservation equations applicable to the flow of a reactive multi-component system. A discussion is also given in this section on the mass, momentum, and heat fluxes of the conservation equations. In Section C, a similarity analysis is performed on the above equations to obtain the dimensionless parameters pertinent to the flow of a reactive mixture. The ranges of the similarity parameters of interest are stated. The chemical kinetic model used in this work is presented in Section D. The boundary layer equations and boundary conditions governing the flow are introduced in Section E along with the approximations used in their derivation. Finally, in Section F the equations are transformed to a set of ordinary differential equations by appropriate transformations.

B. Conservation Equations

In the theory of aerothermochemistry, the fundamental equations governing the flow of a multi-component reacting mixture are: the conservation of species, the conservation of mass, the conservation of

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momentum, the conservation of energy, and the equation of state of the mixture. In general, two different approaches exist for the derivation of the above equations. One approach employs the theory of independent coexistent continua [35]. Each continuum obeys the law of classical mechanics and thermodynamics. In this analysis the concept of control volume and control surface for each continuum is used. A disadvantage of this method is that phenomenological relations between stress and strain, heat flux and temperature gradient, diffusion flux and concentration gradient must be postulated. The alternative approach is that of the kinetic theory of gases [36,37]. From the kinetic theory the transport properties of the mixture can be expressed in terms of collision integrals which are functions of the dynamics of intermolecular collisions. A certain amount of uncertainty occurs in evaluating the above integrals. A comparison of the conservation equations obtained by the two approaches leads to identical results.

The basic conservation equations have been derived by several investigators [35,36,37,38,39,40], with varying degrees of elegance; therefore, in the present work the initial formulation is limited to the introduction of the general form of the equations and the definition of the various terms which appear in these equations. The form of the conservation equations derived by Williams [41] is closely followed.

1. Conservation of Species

The general conservation of species equation is:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla\cdot[\rho Y_i(\vec{v}+\vec{V}_i)] = w_i \qquad i=1,\ldots N \tag{1}$$

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where w_i = net production of mass of species i by chemical reaction per unit volume and time.

The diffusion velocity $\vec{V}_i$ is defined by:

$$\vec{v}_i = \vec{v} + \vec{V}_i$$

and

$$\sum_i^N Y_i \vec{V}_i = 0$$

where $Y_i = \rho_i/\rho$ = mass fraction of species i.

$\vec{v}$ = macroscopic velocity of the mixture.

The diffusion velocity can be considered to be composed of four components resulting from gradients in concentration, temperature, pressure, and external forces, i.e.:

$$\vec{V}_i = \vec{V}_i^{(Y_i)} + \vec{V}_i^{(T)} + \vec{V}_i^{(P)} + \vec{V}_i^{(f_i)} \qquad (2)$$

Hirschfelder *et al.* [37] obtained an expression for the diffusion velocity of dilute gases of the form

$$\vec{V}_i = \frac{n^2}{n_i \rho} \sum_j^N W_j D_{ij} \vec{d}_j - \frac{D_{T,i}}{n_i W_i} \nabla \ell n T \qquad (3)$$

where

$$\vec{d}_j = \nabla X_j + (X_j - Y_j) \nabla \ell n p - \frac{Y_j}{p} \left[\frac{\rho_j}{W_j} \vec{f}_j - \sum_k^N n_k \vec{f}_k \right] \qquad (4)$$

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In the case of a binary mixture where the effects of thermal diffusion, pressure gradient diffusion, and body forces are not important, equation (3) reduces to:

$$\vec{V}_i = \frac{n^2}{n_i \rho} W_j D_{ij} \nabla X_j \tag{5}$$

In terms of mass fraction equation (5) reduces to the well-known Fick's Law:

$$\vec{V}_i = -D_{ij} \nabla \& n Y_i \tag{6}$$

For a multi-component system Fick's Law is applicable when, in addition to the above assumptions, the binary diffusion coefficients of all the species are equal.

2. Overall Continuity

Since mass is neither created nor destroyed by chemical reactions (excluding nuclear reactions), but only transformed from one species to another, then:

$$\sum_i^N w_i = 0 \tag{7}$$

Bearing in mind the definition of the diffusion velocity and equation (7), the summation of equation (1) over all N species results in:

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$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \tag{8}$$

Equation (8) is identical to the continuity equation of a one-component fluid.

3. Conservation of Momentum

The momentum equation of a multi-component reacting mixture is:

$$\rho \frac{\partial \vec{v}}{\partial t} + \rho \vec{v} \cdot \nabla \vec{v} = \nabla \cdot \underline{\pi} + \rho \sum_{i}^{N} Y_i \vec{f}_i \tag{9}$$

The pressure tensor $\underline{\pi}$ may be expressed as a sum of the hydrostatic pressure p, and the viscous stress tensor $\underline{\tau}$, i.e.:

$$\underline{\pi} = -p\underline{I} + \underline{\tau} \tag{10}$$

where $\underline{I}$ is the unit tensor. The viscous stress tensor is given by:

$$\underline{\tau} = \left[\left(-\frac{2}{3}\mu + \kappa\right)\nabla \cdot \vec{v}\right]\underline{I} + \mu[(\nabla \vec{v}) + (\nabla \vec{v})^T] \tag{11}$$

The coefficient of bulk viscosity κ will be taken as zero. Strictly speaking $\kappa = 0$ only for monatomic gases. In multi-component mixtures, an additional term in the pressure tensor expression (10) arises; the diffusion stress tensor $\underline{\tau}^D$ as a result of the relative motion of the species. In most combustion problems (as in this present work), its contribution is negligible.

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4. Conservation of Energy

A general form of the energy equation is:

$$\rho \frac{\partial u}{\partial t} + \rho \vec{v} \cdot \nabla u = -\nabla \cdot \vec{q} - p \nabla \cdot \vec{v} + \underline{\tau} : \nabla \vec{v} + \rho \sum_{i}^{N} Y_i \vec{f}_i \vec{V}_i \qquad (12)$$

The heat flux vector $\vec{q}$ can be broken down in different components, i.e.:

$$\vec{q} = \vec{q}^{(T)} + \vec{q}^{(D)} + \vec{q}^{(Y_i)} + \vec{q}^{(R)} \qquad (13)$$

which represent the contributions of the heat transfer due to temperature gradient ($\vec{q}^{T}$), the relative motion of the species ($\vec{q}^{D}$), the concentration gradient ($\vec{q}^{Y_i}$), and radiation ($\vec{q}^{R}$). The heat flux attributed to the concentration gradient is known as the Dufour effect.

If the radiant heat is neglected, then the heat flux vector $\vec{q}$ may be written as

$$\vec{q} = -k \nabla T + \rho \sum_{i}^{N} h_i Y_i \vec{V}_i + RT \sum_{i}^{N} \sum_{j}^{N} \frac{X_j D_{T,i}}{W_i D_{ij}} (\vec{V}_i - \vec{V}_j) \qquad (14)$$

Neglecting the Dufour effect and substituting the Fick's form of $\vec{V}_i$ we obtain:

$$\vec{q} = -k \nabla T - \rho \sum_{i}^{N} h_i D_{ij} \nabla Y_i \qquad (15)$$

There are two forms of the energy equation that are most often

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useful. One is expressed in terms of the enthalpy of the mixture. Employing the following thermodynamic relation:

$$u = h - p/\rho \tag{16}$$

and substituting equation (15) and the overall continuity (9) in (14) we have:

$$\rho \frac{\partial h}{\partial t} + \rho \vec{v} \cdot \nabla h = \nabla \cdot (k \nabla T - \rho \sum h_i Y_i \vec{V}_i) + \frac{\partial p}{\partial t} + \vec{v} \cdot \nabla p + \underline{\tau} : \nabla \vec{v} + \rho \sum Y_i \vec{f}_i \vec{V}_i \tag{17}$$

In equation (17) the specific enthalpy of the mixture is defined as:

$$h = \sum_{i}^{N} h_i Y_i \tag{18}$$

where

$$h_i = \int_{T_o}^{T} c_{p,i} dT + h_i^o \tag{19}$$

Another alternate form of the energy equation which proved useful in the present work is in terms of the static temperature of the mixture. From equation (17) with the aid of the conservation of species (1) and the overall continuity (9) we have

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$$\rho c_p\left(\frac{\partial T}{\partial t} + \vec{v}\cdot\nabla T\right) = \nabla\cdot\left(\kappa\nabla T - \rho\sum_i^N Y_i\vec{V}_i\int_{T_o}^{T} c_{p,i}dT\right)$$

$$- \sum_i^N w_i h_i^o + \frac{\partial p}{\partial t} + \vec{v}\cdot\nabla p$$

$$+ \underline{\tau}:\nabla\vec{v} + \rho\sum_i^N Y_i\vec{f}_i\vec{V}_i \qquad (20)$$

C. Similarity Analysis

The governing equations of a chemically-reacting mixture in their present state are in a very complex form and are not conducive to a mathematical treatment. One can reduce the complexity of the above equations by disregarding terms which are not important for the particular problem under investigation. Thus a similarity analysis is desired on the governing equations. Certain dimensionless parameters will result from the analysis, which by specifying their ranges (known as a-priori from the experimental set-up) will render certain terms negligible with respect to others.

A similarity analysis on the conservation equations of a multi-component system is a highly complicated problem. For this reason it is assumed that the diffusion velocity of each species is of the same order as the diffusion velocity of a binary mixture given by Fick's Law. Also that the radiant heat flux and Dufour's effect are assumed to be negligible. It is doubtful that the above simplifications will alter the similarity parameters of the corresponding multi-component system.

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The following dimensionless parameters are defined:

$$x^* = x/L \qquad t^* = t/(L/u_o)$$

$$\vec{v}^* = \vec{v}/u_o \qquad c_{p,i}^* = c_{p,i}/c_{p,o}$$

$$\underline{\tau}^* = \underline{\tau}/(\mu_o u_o/L) \qquad k^* = k/k_o$$

$$\vec{f}_i^* = \vec{f}_i/g \qquad h_i^{o*} = h_i^o/q^o$$

$$p^* = p/\rho_o u_o^2 \qquad \vec{V}_i^* = \vec{V}_i/[(D_i)_o/L]$$

$$T^* = T/T_o \qquad w_i^* = w_i/w_o$$

$$\rho^* = \rho/\rho_o \qquad Y_i^* = Y_i$$

where the subscript o denotes a reference state. With these dimensionless parameters, equations (1), (8), (9), and (20) become:

$$\frac{\partial}{\partial t^*}(\rho^* Y_i^*) + \vec{\nabla}^* \cdot \left[\rho^* Y_i^* (\vec{v}^* + \vec{V}_i^*/(Re)(Sc_i))\right]$$

$$= [w_o/(\rho_o u_o/L)] w_i^* \qquad (21)$$

$$\frac{\partial \rho^*}{\partial t^*} + \vec{\nabla}^* \cdot (\rho^* \vec{v}^*) = 0 \qquad (22)$$

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$$\rho^* \frac{\partial \vec{v}^*}{\partial t^*} + \rho^* \vec{v}^* \cdot \nabla^* \vec{v}^* = -\nabla^* p^* + \frac{1}{(Re)} \nabla^* \cdot \underline{\tau}^* + \frac{1}{(Fr)} \rho^* \sum_i^N Y_i^* f_i^* \qquad (23)$$

$$\rho^* c_p^* \left(\frac{\partial T^*}{\partial t^*} + \vec{v}^* \cdot \nabla^* T^* \right) = \frac{1}{(Re)(Pr)} \nabla^* \cdot \left[k^* \nabla^* T^* - \rho^* \sum_i^N \frac{Pr}{(Sc_i)} Y_i^* \vec{V}_i^* \int_{T_o^*}^{T^*} c_{p,i}^* dT^* \right]$$

$$- \left(\frac{q^o}{c_{p,o} T_o} \right) \left(\frac{w_o}{\rho_o u_o / L} \right) \sum_i^N w_i^* (h_i^o)^*$$

$$+ (Ec) \left(\frac{\partial p^*}{\partial t^*} + \vec{v}^* \cdot \nabla^* p^* \right)$$

$$+ \frac{(Ec)}{(Re)} (\underline{\tau}^* \cdot \nabla \vec{v}^*)$$

$$+ \frac{(Ec)}{(Fr)(Re)} \sum_i^N \frac{1}{(Sc_i)} Y_i^* \rho^* \vec{f}_i^* \vec{V}_i^* \qquad (24)$$

where

$$Re = \rho_o u_o L / \mu_o \qquad \text{(Reynolds Number)}$$

$$Fr = u_o^2 / gL \qquad \text{(Froude Number)}$$

$$Sc_i = \mu_o / \rho_o (D_i)_o \qquad \text{(Schmidt Number)}$$

$$Ec = u_o^2 / c_{p,o} T_o \qquad \text{(Eckert Number)}$$

The Froude number is not pertinent in the present study. In free convective flows a more suitable parameter will be the Grashof number.

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$$Pr = c_{p,o}\mu_o/k_o \qquad \text{(Prandtl Number)}$$

The above similarity parameters are well known from the theory of non-reactive multi-component mixtures. They represent a measure of the relative importance, of inertia and viscous forces, kinetic and potential energy, momentum and mass transfer, kinetic and thermal energy, and momentum and heat transfer, respectively. In reacting mixtures two additional variables are required to describe a process: the heat of reaction and a source term describing the kinetics of the mixture. It must be noted that usually in practical systems the kinetics are described by a number of elementary reactions; consequently, an equal number of dimensionless parameters are required. The present analysis was restricted to one overall reaction, which was assumed to be representative of the chemical kinetics of the mixture.

The similarity parameters that characterize the chemical changes in a process are:

$$D_I = w_o L/\rho_o u_o \qquad \text{(First Damköhler Number)}$$

$$D_{II} = q^o/c_{p,o}T_o \qquad \text{(Second Damköhler Number)}$$

A combination of the two numbers results in Damköhler's third similarity group, i.e.

$$D_{III} = D_I \cdot D_{II} = q^o w_o L/\rho_o u_o c_{p,o} T_o$$

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The First Damköhler number, D_I, represents the ratio of the convective time (L/u_o) to the chemical time (ρ_o/w_o). The Second Damköhler number, D_{II}, represents the ratio of the heat addition by chemical reaction (q^o) to the heat addition associated with the convection of enthalpy ($c_{p,o}T_o$). The Third Damköhler number, D_{III}, represents the ratio of the rate of heat addition by chemical reaction ($q^o w_o/\rho_o$) to the rate of heat addition by convection of enthalpy ($u_o c_{p,o} T_o/L$). The above definition of Damköhler's First similarity group is quite general since the reaction source term depends on such quantities as the temperature, the species mass fraction, and the activation energy. A more restricted definition will be given in a later section after discussing the chemical source term.

The low-speed forced convection flow of a gaseous mixture is of great interest in ignition studies by hot surfaces. This flow can be specified in terms of the similarity parameters by considering their order of magnitude in the following ranges:

$$O(Re) >> 1$$

$$O(Ec) << 1$$

The Prandtl number (Pr) and the Schmidt number (Sc), that depend only on the physical properties of the mixture are both of order one. For a flow near a solid boundary which is the case in the present study, the above ranges of the dimensionless parameters indicate:

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a. Prandtl's Boundary Layer approximation is valid.

b. The body forces are negligible.

c. The energy transported by conduction and by diffusion dominates over shear work.

The order of magnitude of the First Damköhler number (D_I) and, consequently of the Third Damköhler number (D_{III}) cannot be specified since it depends on the degree of "reactivity" of the mixture. For $D = 0$ the state of the mixture is said to be frozen and for $D \to \infty$ the mixture is in chemical equilibrium.

D. Chemical Kinetic Model

To complete the formulation of the problem, an expression for w_i, the mass rate of production of species i by chemical reaction per unit volume and time, is required.

In general for a stoichiometric equation of the form

$$\sum_{j=1}^{N} \gamma_j' M_j \rightleftarrows \sum_{j=1}^{N} \gamma_j'' M_j$$

the law of mass action gives the net production rate of species M_i as

$$\dot{(M_i)} = (\gamma_i'' - \gamma_i') \left[k_f \prod_{j=1}^{N} (M_j)^{\gamma_j'} - k_b \prod_{j=1}^{N} (M_j)^{\gamma_j''} \right]$$

where k_f and k_b represent the forward and backward reaction rate constants, M_i represents the chemical species i, and (M_i) designates their molar concentration. The two reaction rate constants are related by the equation

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$$K_c = \frac{k_f}{k_b}$$

where K_c is the equilibrium constant based on the concentrations.

The reaction mechanism of a flame is of a very complex character since it involves a great number of elementary reactions between stable and unstable species. In the case of the combustion of hydrocarbons, several investigators [42,43,44,45] have proposed various combinations of possible reactions by which the true reaction mechanism of a flame can be approximated. These proposed reaction schemes are by no means unique but depend on the particular experimental technique and methodical "guesswork" of the investigator. Due to the uncertainty of the reaction mechanism of the combustion of hydrocarbons, and the lack of accurate experimental data on reaction rates, most analytical works rely on the concept of "overall chemical kinetics." This concept replaces the actual reaction mechanism of the flame by a single reaction between the fuel and the oxidizer. The above simplified concept came under criticism from Levy and Weinberg [46] who tested this scheme for a lean ethylene-air flat flame. It was found that the effective order and activation energy of the reaction changes considerably at low temperatures, while at zones near the maximum heat release the variations are almost imperceptible.

In the present study the interest focuses on only a qualitative relation between the ignition temperature and the physical and chemical properties of the combustible mixture. Consequently, an overall chemical reaction is assumed, and the chemistry of the flame is represented by:

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$$\nu_O M_O + \nu_F M_F \rightarrow \nu_P M_P$$

The reaction rate is assumed to be given by a second order kinetic expression, i.e.:

$$w = B\rho^2 Y_O Y_F \exp[-E/RT] \tag{25}$$

where B = frequency factor of the reaction.

E = Activation Energy of the reaction.

The source term w is related to the individual species source term by the relation:

$$w = -\frac{W_O}{\nu_O W_O} = -\frac{W_F}{\nu_F W_F} = \frac{W_P}{\nu_P W_P} \tag{26}$$

Furthermore, it is assumed that only four species are present in the flame: oxidizer, fuel, inert gases, and products of combustion.

E. Boundary Layer Equations

1. Governing Equations

The steady-state governing equations of a reacting gaseous mixture in the boundary layer of an axisymmetric or two-dimensional body are [47]:

Continuity

$$\frac{\partial}{\partial x}(\rho u r_o^\epsilon) + \frac{\partial}{\partial y}(\rho v r_o^\epsilon) = 0 \tag{27}$$

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where $\epsilon = 0$ for a two-dimensional flow and $\epsilon = 1$ for an axisymmetric flow. The radius of the body in a meridiam plane is $r_o(x)$. The coordinate system employed is shown in Figure 1.

Momentum
x-Component

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} = - \frac{\partial p}{\partial x} + \frac{\partial}{\partial y} \left(\mu \frac{\partial u}{\partial y} \right) \tag{28}$$

y-Component

$$\frac{\partial p}{\partial y} = O(1) \tag{29.a}$$

Although the pressure gradient normal to the wall is of order one, the total pressure change throughout the boundary layer normal to the wall will still be small, or of the order δ, and may be neglected. Thus

$$p = p_e \tag{29.b}$$

The pressure gradient dp_e/dx can be eliminated from the momentum equation by means of the following equation

$$\rho_e u_e \frac{du_e}{dx} = - \frac{dp_e}{dx} \tag{30}$$

which is the momentum equation of the inviscid flow outside the boundary layer.

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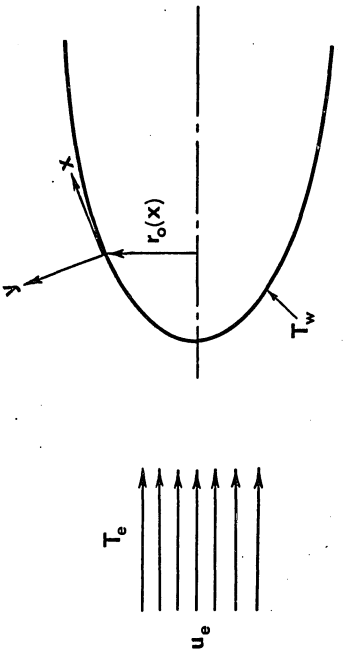

Figure 1. Coordinate System

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Conservation of Reactive Species

$$\rho u \frac{\partial Y_i}{\partial x} + \rho v \frac{\partial Y_i}{\partial y} = \frac{\partial}{\partial y}\left(\rho D_i \frac{\partial Y_i}{\partial y}\right) + w_i \quad \text{for } i=O,F,P \tag{31}$$

Conservation of Inert Gas

$$\rho u \frac{\partial Y_N}{\partial x} + \rho v \frac{\partial Y_N}{\partial y} = \frac{\partial}{\partial y}\left(\rho D_N \frac{\partial Y_N}{\partial y}\right) \tag{32}$$

Energy

$$\rho c_p\left(u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y}\right) = \frac{\partial}{\partial y}\left(k \frac{\partial T}{\partial y}\right) - \sum_i^N \left(\int_{T_O}^T c_{p,i} dT + h_i^O\right) w_i + \sum_i^N \rho D_i c_{p,i} \frac{\partial Y_i}{\partial y} \frac{\partial T}{\partial y} \tag{33}$$

Equation of State

$$p = \rho RT \sum_i^N (Y_i/W_i) \tag{34}$$

For the derivation of the above equations the following assumptions were used:

a. The fluid is made up of a mixture of perfect gases.

b. The flow is laminar and steady-state.

c. The boundary layer approximation is valid.

d. The effects of body forces are negligible.

e. The diffusion velocity is given by Fick's Law, equation (6).

f. The heat flux vector is given by equation (15).

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g. Low-speed flow exists.

In order to bring out the main features of the problem as simply as possible without destroying its physical character, the following additional assumptions will be made:

h. The specific heat at constant pressure for all species is the same and independent of temperature and composition, i.e.:

$$c_{p,i} = c_p = \text{constant}$$

i. The binary diffusion coefficients of all the species are the same, i.e.,

$$D = D_i$$

Assumptions (h) and (i) simplify the energy equation (33) which becomes

$$\rho c_p \left(u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right) = \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) - \sum_{i}^{N} h_i^{o} w_i \qquad (35)$$

2. Boundary Conditions

The boundary conditions of the momentum equation are:

at $y = 0$: $\quad u = 0; \quad v = 0 \qquad (36.a,b)$

at $y \to \infty$: $\quad u \to u_e(x) \qquad (36.c)$

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The value of $u_e(x)$ is determined by the solution of the inviscid flow outside the boundary layer.

The boundary conditions on the conservation of species equations are:

$$\text{at } y = 0: \qquad \frac{\partial Y_i}{\partial y} = 0 \qquad \text{for } i=O,F,N,P \tag{37.a}$$

The above boundary condition states that at the solid interface the diffusion of all species is zero, i.e., the surface is non-catalytic. In the flow outside the boundary layer the species mass fraction will be assumed to have a known value, hence

$$\text{at } y \to \infty: \qquad Y_i \to (Y_i)_e \qquad \text{for } i=O,F,N,P \tag{37.b}$$

For the energy equation the boundary conditions specified are:

$$\text{at } y = 0: \qquad T = T_w \tag{38.a}$$

$$\text{at } y \to \infty: \qquad T \to T_e \tag{38.b}$$

The temperature of the surface, T_w, is assumed constant. The free stream mixture temperature, T_e, has a prescribed and a constant value.

The governing equations and the boundary conditions presented above specify mathematically the problem under investigation. In general, if N is the number of species present in a system, for a

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two-dimensional or axisymmetric geometry, N + 5 differential equations (a continuity equation, two momentum equations, an energy equation, N species conservation equations, and an equation of state) are available with N + 5 unknowns ($u,v,p,\rho,T,Y_1,Y_2 \ldots Y_N$). The total order of the differential equations is 2N + 5 and the number of boundary conditions is 2N + 5.

For the reactive flow of a mixture near the stagnation region of a blunt body, which is presently considered, the governing partial differential equations (subject to appropriate boundary conditions) can be reduced to a set of ordinary differential equations by suitable transformations, regardless of the form of the chemical source term.

F. Self-Similar Equations of the Axisymmetric Stagnation Flow

Consider the following transformation coordinates first introduced by Lees [47]

$$s \equiv \int_0^x \rho_e \mu_e u_e r_o^{2\epsilon} dx \tag{39}$$

$$\eta \equiv [\rho_e u_e/(2s)^{1/2}] \int_0^y r_o^{2\epsilon}(\rho/\rho_e)dy \tag{40}$$

The stream function, ψ, is defined as

$$\psi(s,\eta) = (2s)^{1/2} f(\eta) \tag{41}$$

From the continuity equation

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$$u = u_e f'(\eta) \tag{42}$$

and

$$\rho v = -\rho_e \mu_e u_e r_o^{\epsilon}\left[(2s)^{-1/2} f(\eta) + (2s)^{1/2} \frac{\partial \eta}{\partial s} f'(\eta)\right] \tag{43}$$

Near the stagnation point of a blunt body

$$\begin{aligned} r_o &= x \\ u_e &= ax \end{aligned} \tag{44}$$

The coefficient a in equation (44) is a measure of the convective time (1/a) and its value depends on the geometry of the flow. For an axisymmetric jet ($\epsilon = 1$), impinging on a flat plate, $a = u_\infty/d$ where d is the diameter of the jet.

The transformed governing equations for the axisymmetric flow are:

Momentum

$$(Cf'')' + ff'' = \frac{1}{2}\left[(f')^2 - (\rho_e/\rho)\right] \tag{45}$$

Oxidizer Species Conservation

$$\left(\frac{C}{Sc}\alpha_O'\right)' + f\alpha_O' = \bar{D}_I\left(\frac{1}{\theta}\right)\alpha_O\alpha_F e^{-E^*/\theta} \tag{46}$$

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Fuel Species Conservation

$$\left(\frac{C}{Sc}\,\alpha_F'\right)' + f\alpha_F' = (n_e+1)\bar{D}_I\left(\frac{1}{\theta}\right)\alpha_O\alpha_F e^{-E^*/\theta} \tag{47}$$

Inert Gas Species Conservation

$$\left(\frac{C}{Sc}\,\alpha_N'\right)' + f\alpha_N' = 0 \tag{48}$$

Energy

$$\left(\frac{C}{Pr}\,\theta'\right)' + f\theta' = -(n_e+1)\bar{D}_I\bar{D}_{II}\left(\frac{1}{\theta}\right)\alpha_O\alpha_F e^{-E^*/\theta} \tag{49}$$

The primes denote differentiation with respect to the similarity variable η. The modified Damköhler numbers $\bar{D}_I$ and $\bar{D}_{II}$ are defined as

$$\bar{D}_I = \frac{1}{2}\,\gamma_O W_O Y_{F,e}(B\rho_e/a) \tag{50}$$

$$\bar{D}_{II} = q^O Y_{F,e}/c_{p,e}T_e\gamma_F W_F \tag{51}$$

where $q^O = \sum_i \gamma_i W_i h_i^O$ is the standard heat of reaction. The remaining dimensionless quantities are defined as:

$\theta = T/T_e$ (Dimensionless Temperature)

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$$f' = u/u_e \qquad \text{(Dimensionless Velocity)}$$

$$C = \rho\mu/\rho_e\mu_e$$

$$\alpha_i = Y_i/Y_{i,e} \qquad \text{(Normalized Mass Fraction of Species)}$$

$$E^* = E/RT_e \qquad \text{(Dimensionless Activation Energy)}$$

$$n_e = (Y_{O,e}\nu_F W_F/Y_{F,e}\nu_O W_O) - 1$$

The dimensionless number n_e represents a measure of the "stoichiometry" of the reactants. For $n_e = 0$ the mixture is in stoichiometric composition while for $n_e > 0$ the mixture is lean and for $n_e < 0$ the mixture is rich. The transformed boundary conditions are:

at $\eta = 0$:

$$f = 0; \quad f' = 0; \quad \theta = \theta_W; \qquad (53.a)$$

$$\alpha_i' = 0 \quad \text{for } i=O,F,N,P$$

at $\eta \to \infty$:

$$f' \to 1; \quad \theta \to 1 \qquad (53.b)$$

$$\alpha_i \to 1 \quad \text{for } i=O,F,N,P$$

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CHAPTER IV

THE STEADY-STATE THEORY OF IGNITION OF FLOWING MIXTURES BY HOT SURFACES

A. General Theory

With reference to the dimensionless form of the conservation equations presented in Chapter III, equations (21) - (24), the steady-state solution of a reactive flow in contact with a constant temperature solid boundary can be represented with the following general function of independent dimensionless parameters:

$$\theta = \theta\{\vec{x},(Y_1)_e,(Y_2)_e\ldots(Y_{N-1})_e,Re,Pr,$$

$$(Sc)_1,(Sc)_2\ldots(Sc)_{N-1},D_I,D_{II}, \text{ ratios}$$

$$\text{of physical properties, } \phi(1),\phi(2)\ldots\} \qquad (54.a)$$

where N is the number of species present in the reactive mixture. In the above equation only N - 1 species mass fractions and correspondingly N - 1 Schmidt numbers are required. The Nth species mass fraction is related to the remainder N - 1 species mass fractions by the relation:

$$\sum_{i=1}^{N} Y_{i,e} = 1$$

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In equation (54.a) the reference state (denoted by the subscript e) is taken to be the free stream conditions outside the boundary layer of the solid surface.

All the parameters of equation (54.a) except the ϕ-parameters were derived from the conservation equations of a N-component reactive mixture. The radiant heat transfer, thermal diffusion and other relatively unimportant transport processes were neglected. The chemical source term in the conservation of species equation was expressed by a one-step chemical reaction. This is represented by the First Damköhler similarity parameter. In general, for a multi-step reaction scheme, there exist a number of First Damköhler parameters equal in number to the elementary reactions. Each represents the ratio of the convective time of the system to the chemical time of the particular reaction. However, in certain cases one of the elementary reactions can be considered as the rate-controlling reaction and, therefore, the representation of the chemical kinetics of the system by one parameter is sufficient.

The dimensionless parameters $\phi(1),\phi(2)\ldots$ express the influence of the gas-solid interface on the general solution of the governing equations. Therefore, these parameters can be investigated by considering the transport processes occurring at the interface. Due to the non-catalytic nature of the surface under consideration and the exclusion of any mass-transfer processes at the wall, the only transport process occurring at the interface is the heat transfer. This process, as stated in the Introduction, is of primary importance in the ignition

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studies and, therefore, it should introduce the ϕ-parameters of equation (54.a). If mass transfer or wall catalytic reactions are included, then additional ϕ-parameters must be considered. For example, in the case of a wall-catalytic chemical reaction, the surface Damköhler number will constitute a suitable dimensionless parameter. The inclusion of mass transfer processes at the interface will make the condition on the fluid velocity non-homogeneous, thus introducing another parameter.

Across the interface, heat is transported only by conduction, and according to the theory of one component heat transfer system [48], a suitable parameter to represent the surface heat transfer process is the Nusselt number, Nu. The question arises now, whether the general solution of the conservation equations are influenced by the parameter Nu. It is well known that for a non-reactive one-component flow the Nusselt number is a function of the Reynolds number, and the Prandtl number. For fixed values of Re and Pr the value of Nu remains constant and, therefore, the heat transfer process at the interface of an inert system does not introduce a new similarity parameter.

Penner [49], in deriving the similarity parameters for chemical reactors, had assumed that the Nusselt number's dependence on the Prandtl number and Reynolds number alone, still holds for reactive mixtures. This contrasts with the numerical results obtained by Fay and Riddell [50] on the stagnation point heat transfer of dissociated air. They found that in the case of a non-catalytic wall the surface heat transfer strongly depends on the First Damköhler similarity parameter, whereas for a perfectly catalytic wall, it is virtually

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independent. A sketch of the computed values of $Nu/(Re)^{1/2}$ versus the First Damköhler number for a non-catalytic wall, is shown on Figure 2.

In reactive mixtures, in addition to Prandtl and Reynolds numbers, the Nusselt number also depends on parameters describing the diffusion processes and chemical kinetics. In the case discussed above involving dissociation or recombination processes, the Nusselt number is uniquely defined by the parameters of equation (54.a) with the addition of the wall temperature (which can be considered a ϕ-parameter). Therefore, in such flows the Nusselt number is a superfluous parameter of equation (54.a) since its value is fixed for given values of the other independent parameters.

The ignition process of a combustible mixture in contact with a hot surface, is associated with a strong exothermic reaction. Due to the magnitude of the exothermicity of the reaction in the boundary layer, the temperature increases and consequently the chemical time decreases considerably. The decrease in the chemical time, t_{ch}, can be of several orders of magnitude, since the chemical time is inversely proportional to the exponential of the reciprocal of the temperature. The first Damköhler number is defined with reference to the free stream conditions; therefore, in flows with strong exothermic reactions, this parameter is not a true indication of the local ratio of the chemical time to the convective time [32]. It is necessary, then, to introduce an additional parameter that accounts for the degree of reactivity in the boundary layer. Such a parameter is the Nusselt number. An assessment of the chemical reaction on the boundary

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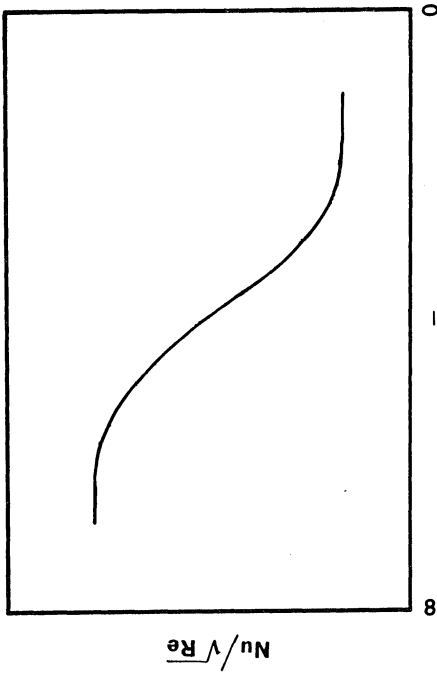

Figure 2. Schematic Representation of a Single-Transition Curve

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layer flow can be specified by the numerical value of the surface heat transfer.

For mixtures with strong exothermic reactions, the general solution of the reactive boundary layer may be given by the expression:

$$\theta = \theta\{\bar{x},(Y_1)_e,(Y_2)_e\ldots(Y_{N-1})_e,Re,Pr,Ec,(Sc)_1,$$

$$(Sc)_2,\ldots(Sc)_{N-1},D_I,D_{II}, \text{ ratios of}$$

$$\text{physical properties, Nu, } \theta_w\} \qquad (54.b)$$

Since the First Damköhler number, directly, and the Nusselt number, indirectly, represent a measure of the reactivity of a mixture, it is natural that they will be the primary parameters in examining the ignition process near a heated wall. From equation (54.b) the Nusselt number can be expressed by the following general relation:

$$Nu = F\{(Y_1)_e\ldots(Y_{N-1})_e,Re,Pr,Ec,(Sc)_1\ldots(Sc)_{N-1},$$

$$D_I,D_{II}, (\text{ratios of physical properties})_w,\theta_w\} \qquad (55)$$

Equation (55) represents the general steady-state criterion for the ignition of a combustible mixture by a hot surface. In the limiting conditions of frozen and equilibrium flows, the Nusselt number becomes independent of the First Damköhler similarity parameter. Thus equation (55) is not valid in these two regions.

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Various simplified forms of the above equation can be obtained by considering a particular region of the flow. For low-speed flows the effects of the Eckert number are insignificant and can be neglected. If, in addition, it is assumed that the diffusion coefficients of the species present are the same and if the variation of the physical properties of the system are neglected, then equation (55) is reduced to:

$$Nu = F\{(Y_O)_e, (Y_F)_e, (Y_N)_e, Re, Pr, Sc, D_I, D_{II}, \theta_w\} \qquad (56.a)$$

In formulating equation (56.a) it has also been assumed that four species are present: oxidizer, fuel, inert gases, and products.

Until now only a general form of the reaction rate law has been considered. If the reaction rate constant is expressed in an Arrhenius form, as is the usual practice in combustion problems, then, the First Damköhler number can be split up into two dimensionless groups: (i) the modified First Damköhler number, $\bar{D}_I$, which includes the pre-exponential term, as shown in equation (50), and (ii) the dimensionless activation energy. With the redefined Second Damköhler number, $\bar{D}_{II}$, equation (51) and the replacement of the fuel and oxidizer mass fraction by the "stoichiometry" ratio equation (56.a) becomes:

$$Nu = F\{Y_{N,e}, n_e, Re, Pr, Sc, \bar{D}_I, \bar{D}_{II}, E^*, \theta_w\} \qquad (56.b)$$

For the particular range of flows under consideration, the ignition temperature $(\theta_w)_{ign}$ is given by:

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$$(\theta_w)_{ign} = \theta_w(Y_{N,e}, n_e, Re, Pr, Sc, \bar{D}_I, \bar{D}_{II}, E^*) \qquad (57)$$

In numerical examples the wall temperature is assumed to be known a priori. A correlation between the surface heat transfer and the First Damköhler number will reveal the influence of the free stream conditions (mixture composition, velocity, and temperature) on the ignition temperature.

In the following section, a specific case is considered to demonstrate the applicability of the First Damköhler number-Surface heat transfer relationship on ignition studies.

B. Ignition Characteristics of a Stagnation-Point Combustible Mixture

The differential equations and boundary conditions governing the axisymmetric, stagnation-point flow of a combustible mixture were derived in Section F of Chapter III.

The conservation of species equations (46) and (47) can be suitably combined and readily integrated to give

$$\alpha_0 = 1 - (1-\alpha_F)/(n_e+1) \qquad (58)$$

The solution of the Inert Gas species equation (48) with the prescribed condition yields:

$$\alpha_N = 1 \qquad (59)$$

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A further reduction of the non-linear equations to be solved is achieved through the use of the following additional assumptions:

j. Lewis number equal to unity.

k. $C = 1$, i.e. $\rho\mu = \rho_e\mu_e$.

Assumptions j and k are a usual practice in combustion theory. The Lewis number (Le) equal to unity assumption, simplifies the problem considerably through the Shvab-Zeldovich formulation. The effect of $Le \neq 1$ on the ignition temperature of premixed gases was found to be unimportant [25].

Equations (47) and (49) can now be combined with the use of assumption j to yield the following linear differential equation:

$$(\alpha_F+\theta/\bar{D}_{II})'' + Prf(\alpha_F+\theta/\bar{D}_{II})' = 0 \qquad (60)$$

Defining a normalized quantity β as

$$\beta \equiv [(\alpha_F+\theta/\bar{D}_{II})-(\alpha_F+\theta/\bar{D}_{II})_w]/[(\alpha_F+\theta/\bar{D}_{II})_e-(\alpha_F+\theta/\bar{D}_{II})_w] \qquad (61)$$

equation (60) reduces to

$$\beta'' + Prf\beta' = 0 \qquad (62)$$

with boundary conditions

$$\beta(0) = 0 \quad \text{and} \quad \beta(\infty) \to 1 \qquad (63)$$

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Before proceeding with the solution of the governing equations, the surface heat transfer will be briefly examined. Using assumption (c), equation (15) becomes

$$q = -k\frac{\partial T}{\partial y} - \rho D \sum_{i=1}^{N} h_i \left(\frac{\partial Y_i}{\partial y}\right) \tag{64}$$

Next, employing the relation

$$d\eta = (2a/\rho_e \mu_e)^{1/2} \rho dy \tag{65}$$

we obtain

$$q = -(2a\rho_e\mu_e)^{1/2} c_p T(C/Pr)\left[\theta' + (Le/c_p T_e) \sum_{i}^{N} h_i Y_{i,e} \alpha_i'\right] \tag{66}$$

For low-speed flow the Nusselt number is defined as

$$Nu = q_w x/k(T_e - T_w) \tag{67}$$

then from equation (66)

$$Nu/(Re)^{1/2} = -(2C_w)^{1/2}\left[\theta' + Le \sum_{i}^{N} h_i Y_{i,e} \alpha_i'/c_{p,w} T_e\right]/(1-\theta_w) \tag{68}$$

where

$$Re = u_e x/(\mu_w/\rho_w) \tag{69}$$

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For a non-catalytic surface, where $dY_i/d\hat{n} = 0$ the gradient of β at the wall is related to the surface heat transfer by the relation

$$q_w = -(2a\rho_e\mu_e)^{1/2} c_p T_e C_w \left(\frac{1}{Pr}\right)[1-\theta_w+\bar{D}_{II}(1-\alpha_{F,w})]\left(\frac{d\beta}{d\eta}\right)_w \qquad (70.a)$$

or

$$Nu/(Re)^{1/2} = -(2C_w)^{1/2}[1-\theta_w+\bar{D}_{II}(1-\alpha_{F,w})]\left(\frac{d\beta}{d\eta}\right)_w/(1-\theta_w) \qquad (70.b)$$

The two extreme values of the surface heat transfer are given for equilibrium flow as $\bar{D}_I \to \infty$ by

$$Nu/(Re)^{1/2} = -(2)^{1/2}(1-\theta_w+\bar{D}_{II})\left(\frac{d\beta}{d\eta}\right)_w/(1-\theta_w) \qquad (71)$$

and for frozen flow as $\bar{D}_I \to 0$ by

$$Nu/(Re)^{1/2} = -(2)^{1/2}\left(\frac{d\beta}{d\eta}\right)_w$$

The value of C_w in equations (71) and (72) was taken to be equal to unity according to assumption (k).

Of greatest interest are the values of the surface heat transfer at the intermediate values of $\bar{D}_I$. These results can be achieved by simultaneously integrating the governing equations for various values of $\bar{D}_I$. Before attempting to solve the compressible boundary layer equations, the incompressible fluid dynamic approximation was considered. This requires a relatively mild numerical effort. Jain and Mucunda [33]

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suggested that fluid dynamic approximations have little effect on the ignition characteristics of reactive flows. They have not considered the case of compressible flow. Thus, the incompressible solution will serve as means of evaluating the above statement.

A second and equally important reason for considering the incompressible case is that its solution will give us a reasonable estimation of the location of the unknown conditions at the wall. This is essential for successful application of an iteration scheme.

Utilizing assumptions j and k, the differential equations that remain to be solved are:

Momentum

a. Incompressible Flow

$$f''' + ff'' = [(f')^2-1]/2 \tag{73.a}$$

b. Compressible Flow

$$f''' + ff'' = [(f')^2-\theta]/2 \tag{73.b}$$

β-Equation

$$\beta'' + Prf\beta' = 0 \tag{62}$$

Energy

$$\theta'' + Prf\theta' = -Pr\bar{D}_I\bar{D}_{II}(n_e+\alpha_r)\alpha_F e^{-E^*/\theta}/\theta \tag{74}$$

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Equation (74) was obtained from equation (49) by substituting the expression for α_0, equation (58).

1. Incompressible Boundary Layer

The momentum equation, subject to the incompressible approximation, is independent of θ and consequently, equations (73.a) and (62) can be solved independently and their solution is then used to solve equation (74) for the entire domain of values of $\bar{D}_I$.

a. Numerical Procedure. To carry out the numerical calculations, the monentum equation (73.a), the β-equation (62), and the energy equation (74), were integrated by the Gill's modified Runge-Kutta fourth-order method. The solution of equation (73) can be found elsewhere [51]. The β-equation, being linear and independent of the energy equation, was solved simultaneously with equation (73.a), using the method of "particular solution" [52,53] to satisfy the boundary condition at infinity (η=7.0). Thus, for the final integration of the governing equations only the energy equation remained as a boundary-value problem.

In order to reduce computation time, the field of integration was divided into two regions. A region near the wall ($0 \leq \eta \leq 2.0$) where the temperature gradient is expected to be steep, and the step size of 0.01 in η was selected for this region. For the remainder of the field ($2.0 < \eta \leq 7.0$) the step size of 0.1 in η was used. It should be noted at this point, that, in the source term of the energy equation, the fuel mass fraction was replaced by a quantity relating it in terms of β, θ and $\alpha_{F,w}$ (the value of the fuel mass fraction at the wall), through the use of equation (61). For a given $\theta'(0)$ the value of $\alpha_{F,w}$ is specified

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since both are related by

$$\theta'(0) = \bar{D}_{II}\beta'(0)[(1+1/\bar{D}_{II})-(\alpha_F+\theta/\bar{D}_{II})_w] + \alpha_{F,w}\bar{D}_{II} + \theta_w \qquad (75)$$

Equation (75) was obtained by differentiating equation (61).

At a given value of $\bar{D}_I$ the energy equation was integrated for $\theta(0) = \theta_w$ and an assumed value of $\theta'(0)$. The resulting value of $\theta(\eta=7.0)$ was then compared to the true boundary condition at infinity, $\theta(\infty) = 1.0$. The temperature gradient at the wall was subsequently adjusted and the integration was repeated until an agreement of 1/10,000 was achieved in the temperature at $\eta = 7.0$. This procedure was repeated for different values of $\bar{D}_I$.

b. Results and Discussion. The numerical computations of the surface heat transfer were carried out for the following values of dimensionless parameters of the governing equations and boundary conditions.

$$Pr = 0.74 \qquad E^* = 67.1366$$

$$\bar{D}_{II} = 6.4452 \qquad n_e = 0.0$$

$$\theta_w = 2.0,\ 2.5,\ 3.0 \text{ and } 3.5$$

These values correspond to the case of an incoming stoichiometric mixture of methane and air at a temperature $T_e = 300°K$ and an activation energy of 40 kcal/g-mole.

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The established results of $Nu/(Re)^{1/2}$ for the range of $\bar{D}_I$ values encompassing the transition from frozen to equilibrium flow are displayed in Figure 3 for the two values of the dimensionless wall temperature θ_w, of 2.0 and 2.5. Both curves can be divided into three regions based on the value of the surface heat transfer: (a) a region of no reaction where the value of $Nu/(Re)^{1/2}$ is minimum, (b) a region of intense reaction where the value of $Nu/(Re)^{1/2}$ is maximum, and (c) a central region where the surface heat transfer is multivalued. In the central region, $Nu/(Re)^{1/2}$ can have one of three values depending on whether the state of the mixture at the wall lies on the "frozen" flow branch A, the equilibrium branch C, or the intermediate branch B (see also Figure 4).

The three regions presented above are separated by two critical values of the Damköhler number specified as $\bar{D}_{I,i}$ and $\bar{D}_{I,e}$. The critical Damköhler number $\bar{D}_{I,i}$ establishes the boundary between the intense reaction zone and the multivalued region, while the critical Damköhler number $\bar{D}_{I,e}$ establishes the boundary between the no-reaction zone and the multivalued region. The parameters $\bar{D}_{I,i}$ and $\bar{D}_{I,e}$ can be referred to as the critical ignition and extinction First Damköhler numbers, respectively, inasmuch as for $\bar{D}_I > D_{I,i}$ the flow is always in equilibrium and for $\bar{D}_I < \bar{D}_{I,e}$ the flow is always frozen.

Although a stability analysis was not attempted in this work, it can be postulated that the solution of the governing equations corresponding to branch B, is unstable [4]. Therefore, depending on which side of the multivalued region the state of the mixture is initially

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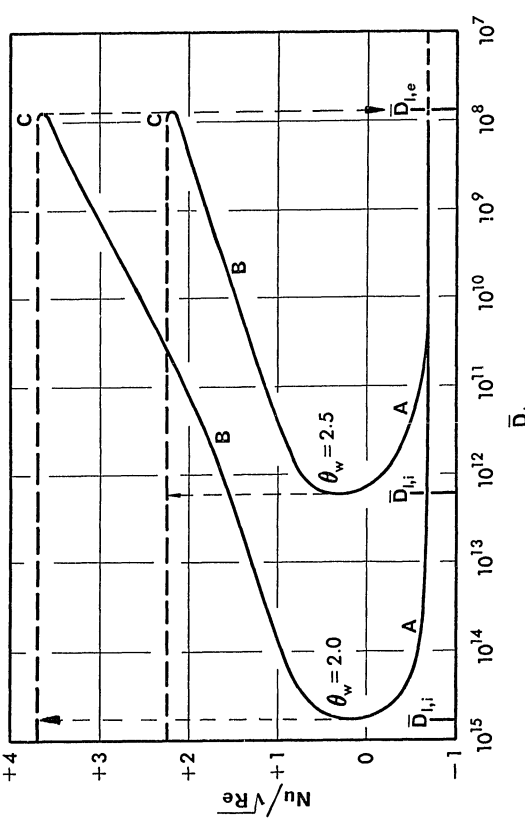

Figure 3. Dependence of the Surface Heat Transfer on the First Damköhler Number

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identified, the surface heat transfer will be given by its value on branch A or C in the multivalued region.

The values of the critical Damköhler numbers for the two wall temperatures considered, are given in Table 1. It is apparent from this comparison that $\bar{D}_{I,i}$ is a strong function of θ_w and $\bar{D}_{I,e}$ is practically independent of θ_w.

Table 1. Critical Damköhler Numbers at Two Wall Temperatures

θ_w	$\bar{D}_{I,i}$	$\bar{D}_{I,e}$
2.0	5.6×10^{14}	7.35×10^{7}
2.5	1.55×10^{12}	7.35×10^{7}

The maximum value of $\bar{D}_I$ for which the flow can be considered frozen varies with the wall temperature. For $\theta_w = 2.0$ and 2.5 the upper limit is $O(10^{13})$ and $O(10^{10})$, respectively. In this range of values of $\bar{D}_I$, the quantity $Nu/(Re)^{1/2}$ is independent of the First Damköhler number and the wall temperature. This is in accord with the familiar Nusselt-Reynolds type equation for non-reactive heat transfer where $Nu/(Re)^{1/2} = f(Pr)$. On the other hand, for branch C, although the parameter $Nu/(Re)^{1/2}$ is independent of $\bar{D}_I$, it is very much dependent on the wall temperature, θ_w. In both the above cases the Nusselt number, Nu, depends on dimensionless parameters that were included in the general solution of the reactive flow, equation (54). Therefore, the surface

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heat transfer does not introduce a new parameter. It must be noted that in the region $\bar{D}_I > \bar{D}_{I,i}$ the surface temperature θ_w must be included in equation (54).

In the intermediate region defined by $\bar{D}_{I,i} \geq \bar{D}_I \geq \bar{D}_{I,e}$ the surface heat transfer is multivalued and the Nusselt number in this region constitutes a ϕ-parameter along with the surface temperature θ_w. This region is the most important in combustion due to the occurrence of two important processes--ignition and extinction. One might explain the ignition mechanism of a combustible mixture by considering the $Nu/(Re)^{1/2}$ versus $\bar{D}_I$ diagram, Figure 3. If the state of the mixture is on branch A (frozen or near-frozen), and $\bar{D}_I$ is increased, the state of the mixture moves along branch A, until it reaches the maximum point defined by $\bar{D}_I = \bar{D}_{I,i}$. If the value of $\bar{D}_I$ is increased still further, so that $\bar{D}_I > D_{I,i}$, then the state of the mixture will "jump" from branch A to branch C. The "jump" from A to C represents the process of ignition. Similarly, with decreasing $\bar{D}_I$ values, the "jump" from C to A will represent the process of extinction.

The normalized fuel mass fraction at the wall plotted against the First Damköhler similarity parameters for two values of the wall temperature $\theta_w = 2.0$ and 2.5 is shown in Figure 4. In a similar manner to the curves in Figure 3, these plots are also divided into the three regions discussed earlier. In the "frozen" region the wall mass fraction of the fuel is unity, while in the equilibrium region, it is zero, signifying complete combustion.

The effect of the wall temperature on $\bar{D}_{I,i}$ is demonstrated in Figure 5.

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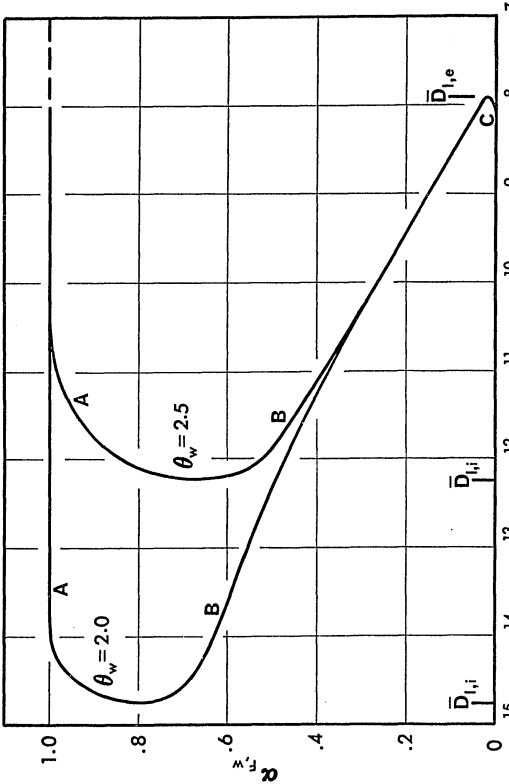

Figure 4. Effect of the First Damköhler Number on the Fuel Mass Fraction at the Wall

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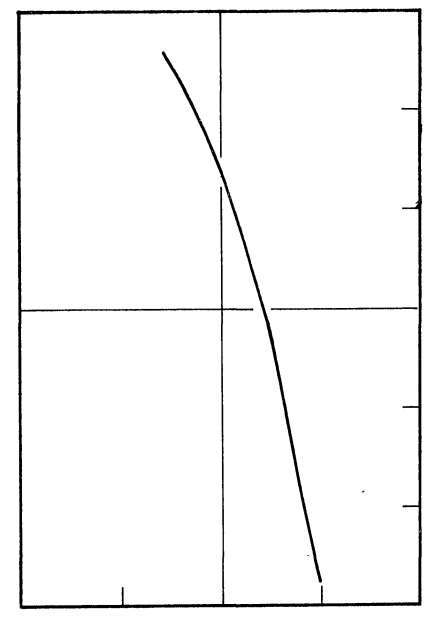

Figure 5. The Influence of the Ignition Temperature on the Critical First Damköhler Number

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For a given fuel mixture $D_{I,i} \propto 1/u_e$ and, therefore, higher free-stream velocities require higher wall temperatures for ignition. For example, from Figure 5, it is evident that ignition may take place at free-stream velocities three orders of magnitude higher for $\theta_w = 2.5$ than it will for $\theta_w = 2.0$.

The temperature distributions in the reactive boundary layer are shown in Figure 6 for different magnitudes of the First Damköhler number. For branch A of the curves in Figure 3, the maximum temperature is at the wall signifying the absence of reaction until the critical ignition First Damköhler number is reached. On branch B on the other hand, a maximum temperature exists at a location away from the wall illustrating the establishment of a reaction region. With decreasing First Damköhler numbers the reaction region moves further away from the solid wall. Finally, Figure 7 represents the normalized fuel concentration profiles. The important fact illustrated by these curves is that the concentration remains constant between the wall and the reaction zone. It is only in the reaction zone that the concentration changes occur, and they reach the free-stream concentrations on the upstream side of the reaction zone.

2. Compressible Boundary Layer

In the case of compressible flow, the momentum equation is temperature dependent and accordingly, the conservation equations must be solved simultaneously. In developing a numerical method for the solution of the governing equations, provisions were made so that the case of Le $\neq$ 1 can be handled if necessary.

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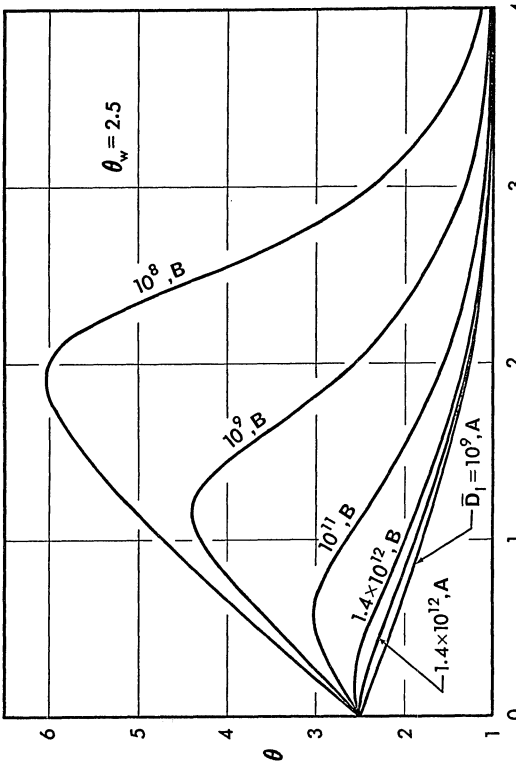

Figure 6. Temperature Profiles

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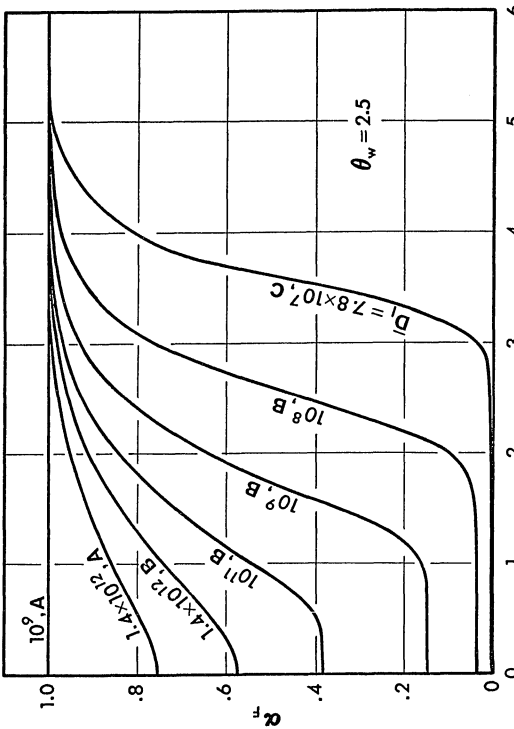

Figure 7. Concentration Profiles

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The governing differential equations are reduced in first order form for numerical computations:

$$\frac{df}{d\eta} = f_1 \tag{76}$$

$$\frac{df_1}{d\eta} = f_2 \tag{77}$$

$$\frac{df_2}{d\eta} = -ff_2 + [(f_1)^2-\theta]/2.0 \tag{78}$$

$$\frac{d\alpha_F}{d\eta} = (\alpha_F)_1 \tag{79}$$

$$\frac{d(\alpha_F)_1}{d\eta} = -Sc[f(\alpha_F)_1-\bar{D}_I(n_e+\alpha_F)a_F e^{-E^*/\theta}/\theta] \tag{80}$$

$$\frac{d\theta}{d\eta} = \theta_1 \tag{81}$$

$$\frac{d\theta_1}{d\eta} = -Pr[f\theta_1+\bar{D}_I\bar{D}_{II}(n_e+\alpha_F)a_F e^{-E^*/\theta}/\theta] \tag{82}$$

The boundary conditions are reduced to

$$\eta = 0: \quad f = 0 \quad ; f_1 = 0;$$

$$(\alpha_F)_1 = 0; \theta = \theta_w$$

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$$\eta \to \infty: \qquad f_1 \to 1; \qquad \theta \to 1; \qquad \alpha_F \to 1$$

The initial value method (shooting) considered here consists of assuming the remaining boundary conditions, e.g., at the wall, necessary to integrate the first order differential equations (76) to (82) and devising an iterative procedure. This procedure adjusts the assumed initial conditions in such a way that the solution of the equations at the edge of the boundary layer tends to approach the free-stream boundary conditions at a prescribed degree of accuracy.

a. Initial Value Method. Let

$$\left.\begin{aligned} s_1 &= f_2(0) \\ s_2 &= \alpha_F(0) \\ s_3 &= \theta_1(0) \end{aligned}\right\} \tag{83}$$

Values of s_1, s_2, and s_3, are sought such that $f(s_1,s_2,s_3,\eta)$, $\alpha_F(s_1,s_2,s_3,\eta)$ and $\theta(s_1,s_2,s_3,\eta)$ are solutions of the original boundary value problem. This will be true only if s_1, s_2, and s_3 are roots of the following system of equations

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$$\left.\begin{aligned} f_1(s_1,s_2,s_3,\infty) - 1 &= 0 \\ \alpha_F(s_1,s_2,s_3,\infty) - 1 &= 0 \\ \theta(s_1,s_2,s_3,\infty) - 1 &= 0 \end{aligned}\right\} \tag{84}$$

Let s_1', s_2', s_3' denote the roots of the above system of equatins. Now since

$$s_i = s_i[f_1(\infty),\alpha_F(\infty),\theta(\infty)] \qquad i=1,2,3 \tag{85}$$

Then using Taylor's expansion theorem we have

$$s_i - s_i' = \frac{\partial s_i'}{\partial f_1(\infty)}[f_1(\infty)-1] + \frac{\partial s_i'}{\partial \alpha_F(\infty)}[\alpha_F(\infty)-1] + \frac{\partial s_i'}{\partial \theta(\infty)}[\theta(\infty)-1] \tag{86}$$

$$i=1,2,3$$

In an iterative procedure, equation (86) may be written as

$$s_i^k = s_i^{k+1} + \frac{\partial s_i^{k+1}}{\partial f_1(\infty)}[f_1(\infty)-1] + \frac{\partial s_i^{k+1}}{\partial \alpha_F(\infty)}[\alpha_F(\infty)-1] + \frac{\partial s_i^{k+1}}{\partial \theta(\infty)}[\theta(\infty)-1] \tag{87}$$

$$i=1,2,3$$

By evaluating the system of equations (87) for four sets of assumed boundary conditions at the wall (keeping the true boundary

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conditions in each case the same), the partial derivatives of the above system may be eliminated to obtain the improved values s_i^{k+1}. Discarding one set of values of s_i^k in favor of the improved set s_i^{k+1} the above described procedure may be repeated until a prescribed accuracy of the system of equations (84) is realized.

b. Numerical Integration. The numerical solution of the compressible case was obtained by means of the Runge-Kutta fourth-order integration method. The above described initial value procedure was used to satisfy the free-stream boundary conditions. The incompressible solution for the same $\bar{D}_I$ values was utilized to estimate the initial four sets of assumed boundary conditions. In the frozen region the iterative procedure converged very rapidly. However, near equilibrium region, the incompressible solution was not close enough to the true solution for the iterative procedure to converge. This was especially apparent when the higher wall temperature (θ_w=3.0) was used in the numerical computations. The failure of the iterative procedure demonstrated the strong dependence of the values of $f'(\infty)$, $\alpha_F(\infty)$ and $\theta(\infty)$ on the boundary conditions at the wall. The difficulty of predicting reasonable estimations of the roots of equations (84) was circumvented by the "variable parameter" method. In this case the parameter is the First Damköhler number $\bar{D}_I$. When a solution was obtained for a given value of $\bar{D}_I$ (e.g. at the frozen region), a small change in the value of the parameter was made, and the neighboring solution was obtained. The formal solution was used as an initial estimated of the roots of equation (84). This procedure was repeated for the entire domain of $\bar{D}_I$ considered.

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c. A Comparison of the Compressible and Incompressible Fluid Dynamic Assumptions.

i. *Critical Ignition First Damköhler Number.* The effect of the incompressible approximation on the critical ignition First Damköhler number is shown in Figures 8 and 9 for two values of the wall temperature, θ_w of 2.5 and 3.0. The incompressible approximation underestimates the value of the above critical parameter by 12 per cent and 20 per cent for $\theta_w = 2.5$ and 3.0, respectively. Thus, for engineering estimations the incompressible results are sufficiently accurate to avoid the extensive numerical effort required for the solution of the compressible reactive boundary layer.

ii. *Velocity Distribution.* A Comparison of the velocity profiles is shown in Figure 10. In the compressible case, due to a considerable decrease in the density of the mixture in the reaction region, the velocity exceeds its free-stream value. This is more pronounced in the unstable region B, where for $\theta_w = 2.5$, the velocity has a maximum value of about 30 per cent higher than at the edge of the boundary layer.

iii. *Skin Friction.* The effect of chemical kinetics and compressibility on the skin friction is illustrated in Figure 11 which is a plot of f"(0) versus the First Damköhler number. The effects of chemical kinetics on the skin friction can be assessed by comparing the value of f"(0) for a given wall temperature at different values of $\bar{D}_I$.

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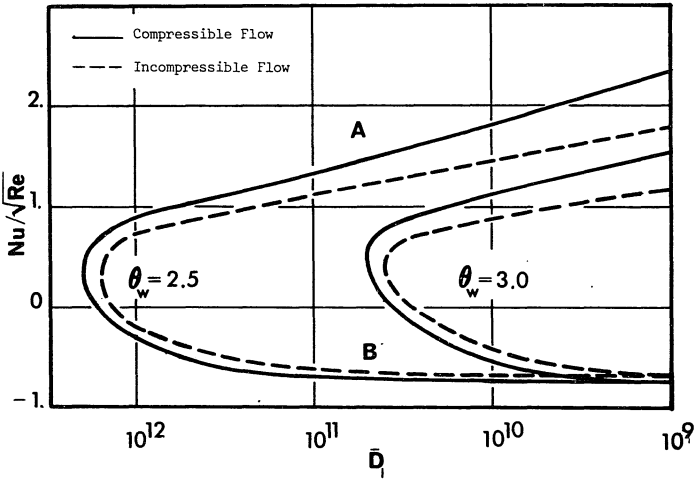

Figure 8. Comparison of Compressible and Incompressible Flows--$Nu/(Re)^{1/2}$ Versus $\bar{D}_I$

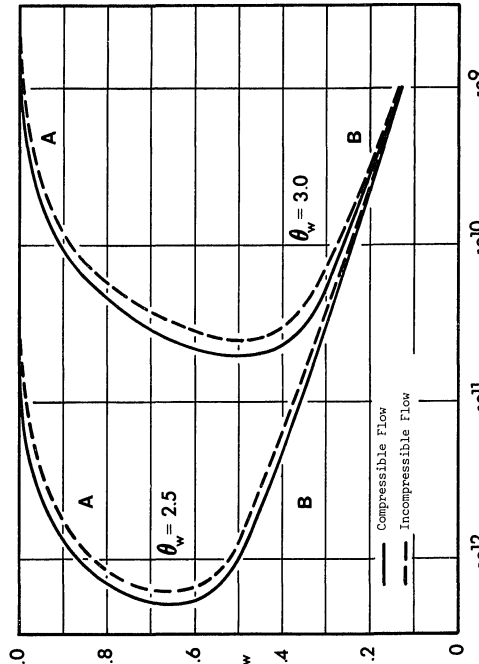

Figure 9. Comparison of Compressible and Incompressible Flows--$\alpha_{F,w}$ Versus $\bar{D}_I$

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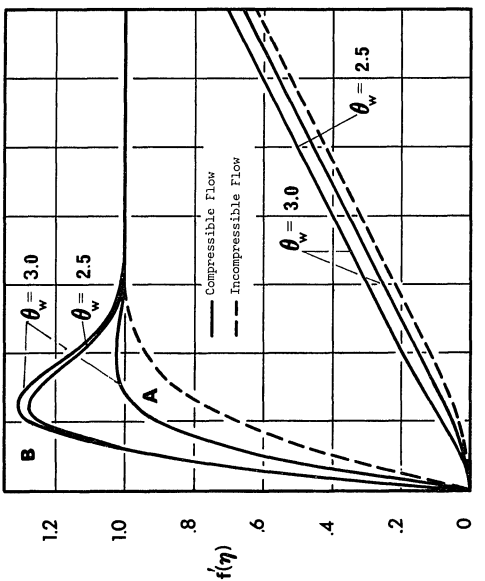

Figure 10. Comparison of Compressible and Incompressible Flows--Velocity Profiles

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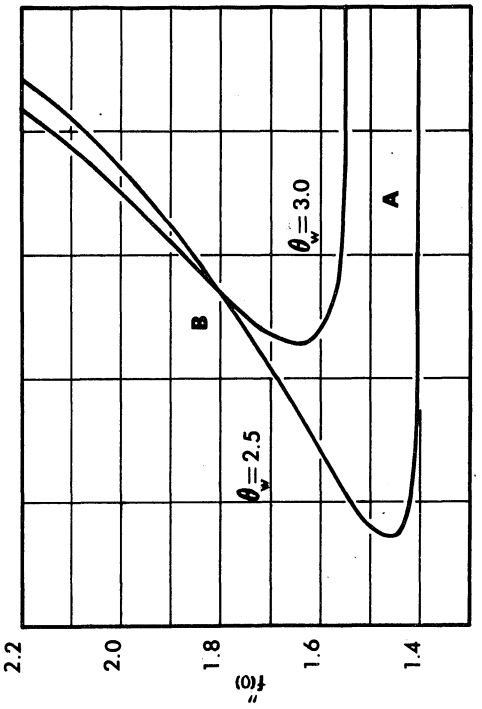

Figure 11. Plot of f''(0) Versus $\bar{D}_I$

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For frozen flow ($\bar{D}_I \leq 10^8$) and $\theta_w = 3.0$ $f''(0) \approx 1.55$), whereas at the same wall temperature and $\bar{D}_I = \bar{D}_{I,i}$ (just prior to ignition), $f''(0) \approx 1.65$.

The effects of compressibility can be studied by considering the values of $f''(0)$ in the frozen region. In the incompressible flow $f''(0) \approx 0.93$, whereas in the compressible flow $f''(0) \approx 1.4$ and 1.55 for $\theta_w = 2.5$ and 3.0, respectively.

iv. *Temperature Distribution.* The temperature distribution variation, due to the incompressible approximation, is illustrated in Figures 12 (θ_w=2.5; $\bar{D}_I$=10^9), 13 (θ_w=3.0; $\bar{D}_I$=10^9) and 14 (θ_w=3.0; $\bar{D}_I$=10^{10}). The following observations for the incompressible solutions referenced to the compressible approximation, are common to these Figures:

a. Predict lower maximum temperature.

b. Predict that the reaction region is further from the wall.

c. Predict a smaller thermal boundary layer thickness.

d. Predict a higher temperature in the frozen branch, whereas in branch B, they predict lower temperatures in the region between the wall and the reaction zone and higher temperatures between the reactin zone and the free stream.

v. *Heat Transfer.* The effect of the incompressible approximation on the surface heat transfer is shown in Figure 8 where the parameter $Nu/(Re)^{1/2}$ is plotted against $\bar{D}_I$, for values of θ_w equal to 2.5 and 3.0. At both temperatures the incompressible fluid dynamic assumption predicts lower values of the surface heat transfer.

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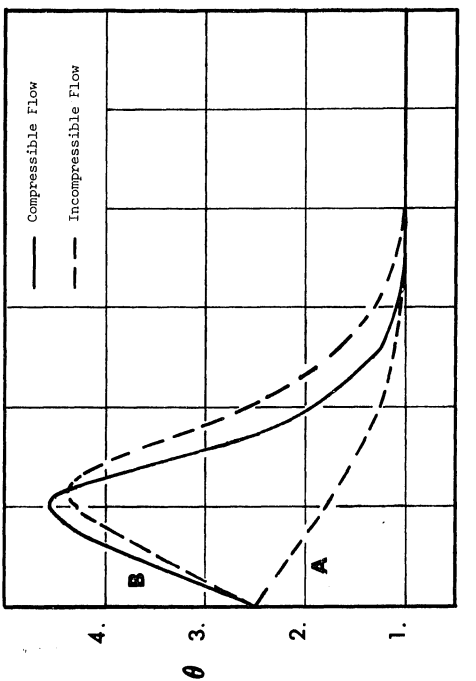

Figure 12. Comparison of Compressible and Incompressible Flows--Temperature Profiles ($D_I=10^9$, $\theta_w=2.5$)

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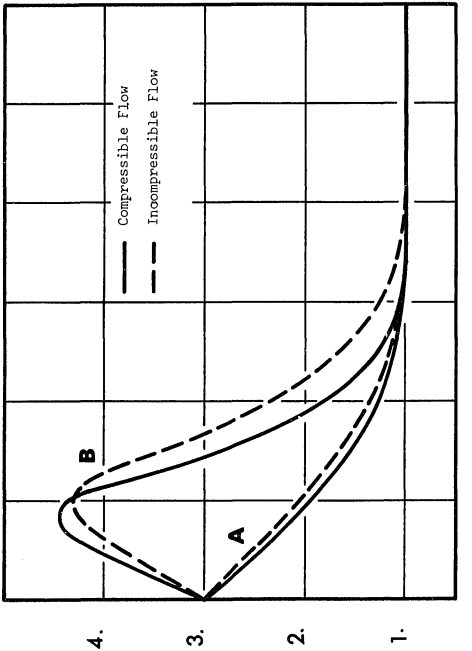

Figure 13. Comparison of Compressible and Incompressible Flows--Temperature Profiles ($D_I=10^3$, $\theta_w=3.0$)

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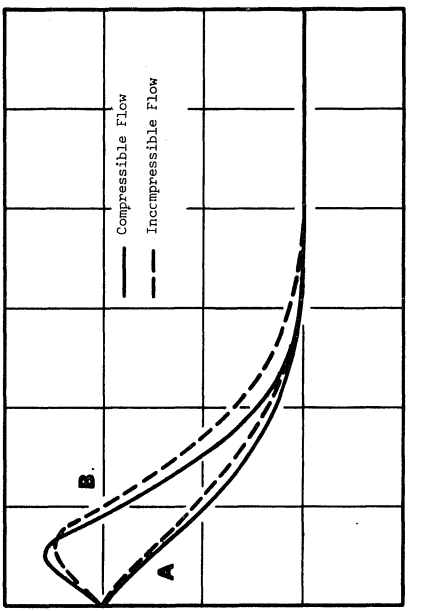

Figure 14. Comparison of Compressible and Incompressible Flows--Temperature Profiles ($D_I=10^{10}$, $\theta_w=3.0$)

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This effect is more pronounced on branch B of the curves, where the surface heat transfer is underestimated by as much as 25 per cent.

vi. *Concentration Distribution.* Figure 15 shows a comparison of the fuel mass fraction distribution for a fixed First Damköhler number and a fixed wall temperature. In the near-frozen region, the incompressible approximation gives lower values of the fuel mass fraction, whereas in region B, near the wall, it gives higher values.

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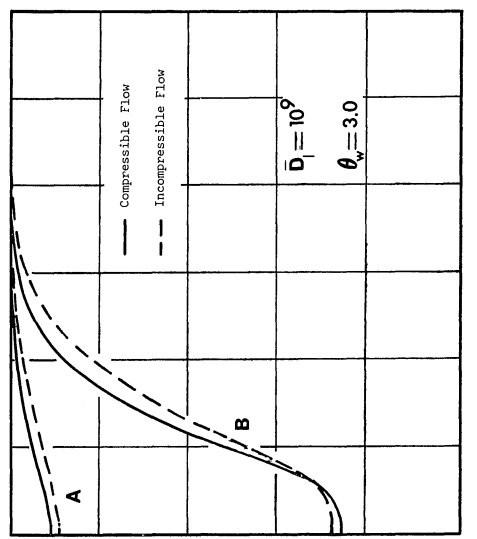

Figure 15. Comparison of Compressible and Incompressible Flows--Concentration Profiles

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CHAPTER V

APPROXIMATE THEORY OF IGNITION: THE VAN'T HOFF CRITERION

The ignition characteristics of a cold combustible mixture at the forward stagnation region of a blunt body will now be examined, using the Van't Hoff criterion, $\partial T/\partial \hat{n} = 0$. In Section A, the ignition characteristics of the above flow are presented where the results were obtained by numerically integrating the governing equations. The ignition criterion was introduced into the problem as an additional boundary condition. The "primary" boundary condition is the temperature of the solid surface (the ignition temperature) which is constant. However, the ignition temperature is considered unknown and must be determined. With the inclusion of the additional boundary condition, the ignition temperature was treated as an eigenvalue.

In Section B, a simplified model, which was developed based on the concept of a reduced film of stationary gases close to the surface of the body, is presented.

A. "Exact" Method

1. Governing Equations and Boundary Conditions

The differential equations governing the flow are identical with those of Chapter IV with the incompressible approximation. For easily accessible reference, they are given below in the most suitable form for the purpose at hand.

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Momentum

$$f''' + ff'' = \frac{1}{2}[(f')^2 - 1] \tag{73}$$

Energy

$$\theta'' + Prf\theta' = -Pr\bar{D}_I\bar{D}_{II}\left[\frac{1}{\theta}\right](n_e+\alpha_F)\alpha_F e^{-E^*/\theta} \tag{74}$$

Linear Combination of Temperature and Mass Fraction

$$(\alpha_F+\theta/\bar{D}_{II})'' + Prf(\alpha_F+\theta/\bar{D}_{II})' = 0 \tag{60}$$

The boundary conditions are

$$\text{at } \eta = 0: \qquad f = f' = 0; \quad \alpha_F' = 0$$

$$\theta = \theta_w \quad ; \quad \theta' = 0 \quad \text{(Ignition Criterion)} \tag{89}$$

$$\text{at } \eta \to \infty: \qquad f' \to 1 \quad ; \quad \alpha_F \to 1$$

$$\theta \to 1 \tag{89}$$

The solution of equation (60), subject to the prescribed boundary conditions is

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$$\alpha_F + \theta/\bar{D}_{II} = 1 + 1/\bar{D}_{II} \tag{90}$$

When the fuel mass fraction at the wall vanishes, i.e., $\alpha_{F,w} = 0$, the temperature at the wall achieves a maximum value and thus, from equation (90)

$$\theta_m = 1 + \bar{D}_{II} \tag{91}$$

Therefore, the range of temperatures at the wall have an upper limit given by equation (91). This is equal to the adiabatic flame temperature of the combustible mixture.

With the aid of equations (90) and (91), the energy equation becomes:

$$\theta'' + Pr f\theta' = -Pr\left(\frac{\bar{D}_I}{\bar{D}_{II}}\right)\left(\frac{1}{\theta}\right)(n_e\bar{D}_{II}+\theta_m-\theta)(\theta_m-\theta)e^{-E^*/\theta} \tag{92}$$

2. Method of Solution

The momentum equation (73) and the energy equation (92) were simultaneously integrated by means of Gill's modified Runge-Kutta fourth order numerical method. The solution of the momentum equation is well known. Thus, the momentum equation was converted to an initial value differential equation using the known third boundary condition at the wall.

A step size of 0.1 in η was used for the numerical solution. Given a value of $R_D = \bar{D}_I/\bar{D}_{II}$ the forward numerical integration of the

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energy equation was performed by using the critical ignition condition $d\theta(0)/d\eta = 0$ and an assumed value of the wall temperature. The resulting value of θ was then compared with the true boundary condition. A trial and error adjustment in the wall temperature with variable step size was used to obtain the ignition temperature for which the corresponding true boundary condition (θ_e=1+0.0001) is achieved.

3. Results and Discussion

The primary calculations were performed for the case of an incoming stoichiometric mixture of methane and air at a temperature T_e = 300°K and an activation energy of 40 kcal/g-mole. The following data were used in the computations:

q^o = 191.579 kcal/g-mole of CH_4.

ρ_e = 0.0013 g/cm^3; $c_{p,e}$ = 0.341 cal/g°K.

Pr = 0.74; p = 1 atm.

For the determination of the effect of inert gas concentration on the ignition temperature, the following values were assigned to the nitrogen mass fraction in the free stream mixture: 0.4, 0.7247 (air), 0.85. Additional calculations were made for values of the activation energy taken at 20 and 30 kcal/g-mole. The effect of the variation of the initial temperature of the mixture was also treated by examining the ignition temperature behavior of methane-air mixture for T_e = 300°K and 500°K.

The qualitative effects of the First Damköhler number $\bar{D}_I$ on the ignition temperature, θ_w, are illustrated in Figure 16. The figure plots R_D defined by equation (93) against the dimensionless ignition

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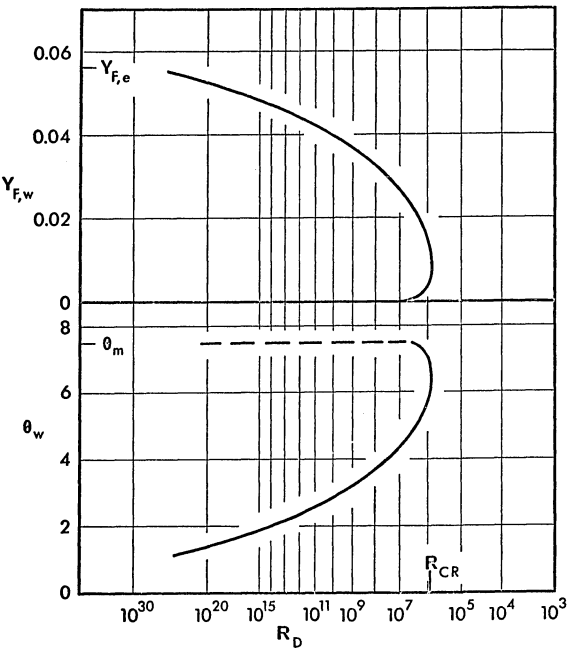

Figure 16. Effect of Variation of D_I on Ignition Temperature and Fuel Mass Fraction at the Wall (T_e=300°K, E=40 kcal/g-mole °K, $Y_{N,e}$=0.7247)

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temperature, θ_w, in the lower scale and against the mass fraction of fuel at the wall, $Y_{F,w}$, in the upper scale. Changes in the parameter R_D here signify changes in $\bar{D}_I$ since $\bar{D}_{II}$ remains constant in the numerical solutions carried out for these plots.

The lower portion of the θ_w-curve represents the ignition temperature, which increases with decreasing values of $\bar{D}_I$. Thus, when the convection time is much larger than the chemical time, represented by large $\bar{D}_I$ values, the plate temperature required to achieve ignition is very low. As the convective time approaches the order of the chemical time, the ignition temperature becomes very high. If one moves along the ignition temperature curve (lower portion of the θ_w-curve) towards lower D_I values, a critical value of this parameter is reached. Since for a given type of fuel and oxidizer, $\bar{D}_I$, is inversely proportional to the velocity of the mixture, then an upper limit on the velocity of the mixture exists, beyond which, irrespective of the flat plate temperature, ignition cannot occur. The limit is designated as R_{CR} on Figure 16. This agrees qualitatively with Patterson's [13,14] experimental results on the ignition of gaseous mixtures by spherical particles.

The validity of the Van't Hoff's ignition criterion is demonstrated in Table 2. In this table, the ignition temperatures obtained using the steady-state theory of ignition developed in Chapter IV, are compared to those obtained by means of the Van't Hoff criterion.

It is evident that employing the Van't Hoff criterion to obtain the ignition temperature is a good approximation. However, it must be

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noted that at low values of the First Damköhler number (high velocities) the Van't Hoff criterion underestimates the ignition temperatures.

Table 2. Comparison of the Ignition Temperatures

$D_{I,i}$	θ_w	θ_w (Van't Hoff Criterion)
5.6×10^{14}	2.0	2.0
1.55×10^{12}	2.5	2.5
3.95×10^{10}	3.0	2.9
3.52×10^{9}	3.5	3.3

Returning to Figure 16, the upper portion of the θ_w-curve represents a second solution of the problem with the prescribed boundary condition $d\theta(0)/d\eta = 0$. This boundary condition also represents the condition of an adiabatic wall. Consequently, this portion of the curve represents the burning of the mixture under adiabatic wall conditions and the temperature specifies the adiabatic wall temperature. Again, if one moves along the upper portion of the θ_w-curve towards lower $\bar{D}_I$ values, the same critical Damköhler number is reached. This time the limit represents extinction for the burning mixture under adiabatic wall conditions. The other side of the curve, with decreasing $\bar{D}_I$, asymptotically will approach the adiabatic flame temperature.

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The top curve in Figure 16 represents the fuel mass fraction, $Y_{F,w}$ at the wall for different $\bar{D}_I$ values. This curve is also composed of two parts. The upper portion of this $Y_{F,w}$ curve represents fuel mass fractions at the wall for corresponding ignition temperatures and the values of $Y_{F,w}$ decrease with decreasing $\bar{D}_I$ values until the critical First Damköhler number is reached. Beyond this point the lower section of the $Y_{F,w}$ curve corresponds to the adiabatic wall solution. Note that this portion of the curve in the limit will reach $Y_{F,w} = 0$ as θ_w approaches the adiabatic flame temperature with decreasing values of $\bar{D}_I$.

For comparative purposes, a second fluid-mechanical assumption was considered:

$$[(f')^2-(\rho_e/\rho)] = 0 \tag{94}$$

Lees [47] used this assumption for a highly-cooled stagnation boundary flow where $\rho_e/\rho_w = 0$. Figure 17 shows a comparison of the two approximations made in the solution of the momentum equation. Curve A was obtained using the incompressible approximation and curve B using Lees' approximation. The largest difference exists at the low Damköhler number, representing the high free-stream velocities, while the difference between the two cases diminishes as the Damköhler number increases. It should be noted here that the difference in the critical Damköhler number is about 20 per cent.

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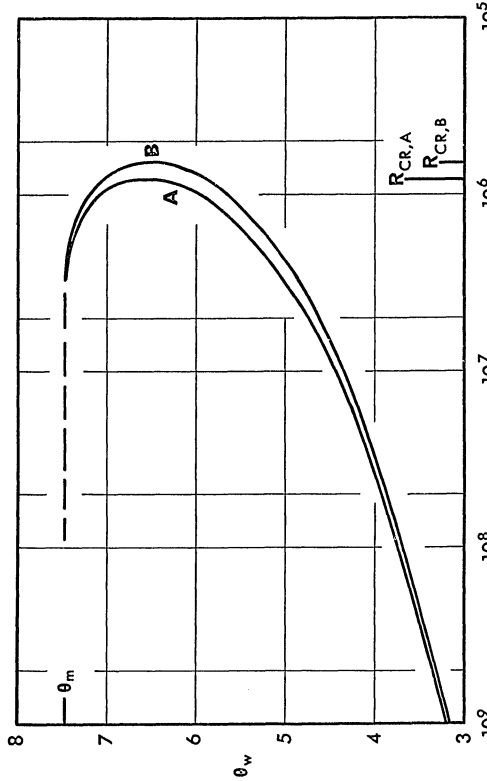

Figure 17. Comparison of Two Approximations:
A. Incompressible Case
B. Lees' Approximation

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The dimensionless temperature profiles of the mixture at ignition temperature are shown in Figure 18. Here the three different values of nitrogen mass fraction in the free-stream composition are represented. The First and Second Damköhler numbers and the dimensionless activation energy were kept constant for the three cases. As was expected, the effect of the presence of nitrogen in larger quantities, was to increase the ignition temperature represented at $\eta = 0$ in this figure.

The effect of the free stream temperature of the mixture on the ignition temperature is shown in Figure 19. The temperature profiles are shown in degrees Kelvin for proper comparison of the results from two different free stream temperatures. These calculations were made for a stoichiometric mixture of methane and air at a specified velocity. Two points are significant from this comparison. First, it should be noted that a decrease in the mixture temperature results in an increase in the ignition temperature. This is in accord with the experimental observations of Mullen *et al.* [15] on the ignition of flowing gaseous mixtures by heated cylindrical rods. Secondly, it appears that a reduction of 200°K in the mixture temperature brings about a comparable increase in the ignition temperature (130°K).

Finally, Figure 20 illustrates the effects of the activation energy on the ignition temperature. Here again, the dimensionless ignition temperatures are plotted against R_D, which as discussed earlier, is directly proportional to the First Damköhler number.

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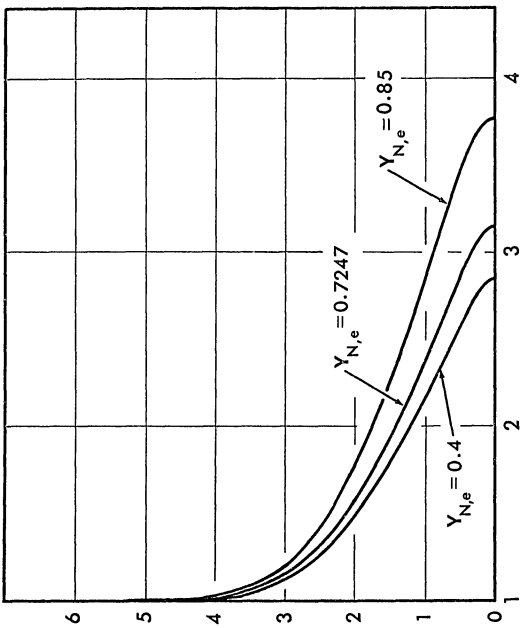

Figure 18. Temperature Distribution and Ignition Temperatures for Various Nitrogen Concentrations

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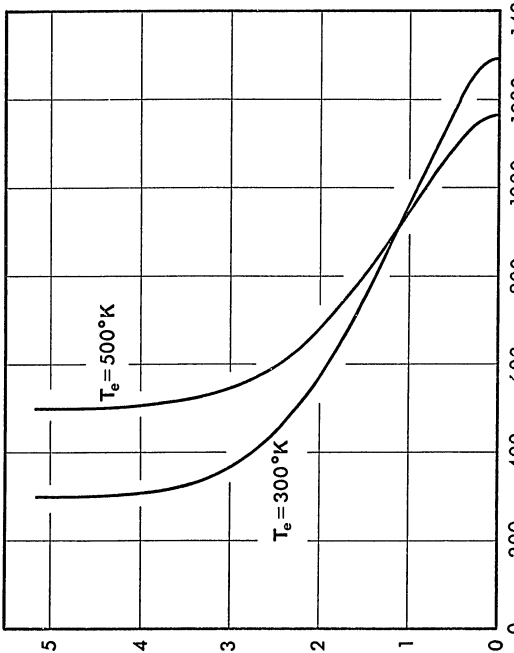

Figure 19. Temperature Distribution and Ignition Temperatures at Two Different Free-Stream Temperatures

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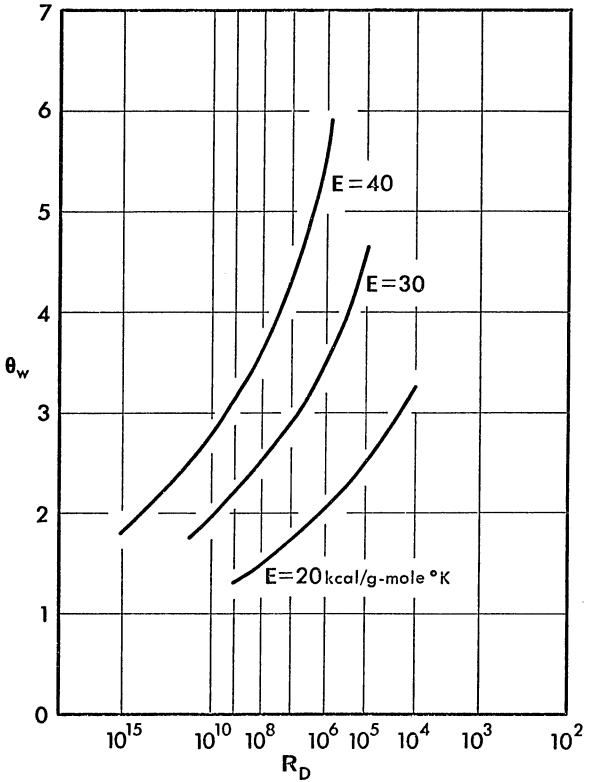

Figure 20. Effect of the Activation Energy on the Ignition Temperatures (T_e=300°K, $Y_{N,e}$=0.7247)

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As expected for a given $\bar{D}_I$ value of the mixture, the higher activation energy requires a higher ignition temperature.

The discussion that follows, although qualitative in nature, will attempt to attribute the above numerical results to the physical concepts governing the problem.

Ignition of the premixed gases occurs when the energy supplied by the heated surface is enough to bring the chemical reaction to a self-accelerating state. The total energy imparted to the mixture is proportional to the product of the time of residence t_r of a gas particle in the heated area and the temperature difference at the wall and free stream. Since the free stream velocity of the mixture is proportional to the time of residence t_r, then for given free stream conditions (excluding the velocity), higher velocities will require higher ignition temperatures.

In the presence of inert gases a given amount of the energy provided by the heated body is used to increase their temperature as well as a quantity of the heat generated by the chemical reaction. Thus the introduction of inert gases impedes ignition.

The increase in the free-stream temperature of the mixture facilitates ignition since the heat losses from the heated region are reduced (smaller temperature gradients).

Finally, lower activation energies bring about lower ignition temperatures since the energy required by the mixture to overcome the "energy barrier", is less.

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B. Simplified Model

To develop a simplified model which will describe the ignition process of a premixed gas by a hot surface; the following two primary assumptions were made: (1) the reaction occurs in a thin film at rest near the wall. The temperature drop across the "stagnant film" is $T_w - T_e$; (2) the heat transfer by convection is independent of the chemical reaction and is given by the product of a convection coefficient which is a function of the free-stream velocity of the mixture and the temperature drop across the "stagnant film."

The conservation equations of the "reduced layer" are:

Energy

$$\frac{d}{dy}\left(k\frac{d\theta}{dy}\right) = -q^{o}\left(\frac{1}{T_e}\right)B\rho^{2}Y_{O,e}Y_{F,e}\alpha_{O}\alpha_{F}e^{-E^{*}/\theta} \tag{95}$$

Conservation of Fuel Species

$$\frac{d}{dy}\left(\rho D\frac{d\alpha_F}{dy}\right) = \nu_F W_F B\rho^{2}Y_{O,e}\alpha_{O}\alpha_{F}e^{-E^{*}/\theta} \tag{96}$$

Conservation of Oxidizer Species

$$\frac{d}{dy}\left(\rho D\frac{d\alpha_O}{dy}\right) = \nu_O W_O B\rho^{2}Y_{F,e}\alpha_{O}\alpha_{F}e^{-E^{*}/\theta} \tag{97}$$

The boundary conditions of the above differential equations are

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at y = 0: $$\theta = \theta_w \tag{98.a}$$

$$\frac{d\alpha_F}{dy} = \frac{d\alpha_O}{dy} = 0 \tag{98.b}$$

at y = δ $$\theta = 1 \tag{99.a}$$

$$\alpha_F = \alpha_O = 1 \tag{99.b}$$

The biggest contribution of the reaction is assumed to be near the wall where the temperature is the highest. Equation (95) is integrated with respect to the temperature between the limits θ_w and 1, and

$$\frac{1}{2}\left[\left[\left(\frac{d\theta}{dy}\right)_w\right]^2 - \left[\left(\frac{d\theta}{dy}\right)_e\right]^2\right] \simeq \frac{q^o B \rho_w Y_{O,e} Y_{F,e} \alpha_{O,w} \alpha_{F,w}}{k_w T_e} \int_1^{\theta_w} e^{-E^*/\theta} d\theta \tag{100}$$

The integral of equation (100) can be written as

$$\int_1^{\theta_w} e^{-E^*/\theta} d\theta = \int_1^{\theta_w} e^{-E^*/[\theta_w(1-(\theta_w-\theta)/\theta_w)]} d\theta \tag{101}$$

and in the first approximation it gives

$$\int_1^{\theta_w} e^{-E^*/\theta} d\theta \simeq \int_1^{\theta_w} e^{-E^*(1+(\theta_w-\theta)/\theta_w)/\theta_w} d\theta \tag{102}$$

which when integrated becomes

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$$\int_1^{\theta_w} e^{-E^*/\theta} d\theta \simeq e^{-E/\theta_w} \frac{\theta_w^2}{E^*} \left[1-e^{-E^*(\theta_w-1)/\theta_w^2}\right] \simeq \frac{\theta_w^2}{E^*} e^{-E^*/\theta_w} \qquad (103)$$

The temperature gradient at the "free" boundary of the reduced film is assumed to be zero and equation (100) with the aid of equation (103) reduces to

$$\frac{1}{2}\left[\left(\frac{d\theta}{dy}\right)_w\right]^2 \simeq \frac{q^o B \rho_w^2 Y_{O,e} Y_{F,e} \theta_w^2}{k_w T_e E^*} \alpha_{O,w} \alpha_{F,w} e^{-E^*/\theta_w} \qquad (104)$$

Let q_{ch} be the surface heat transfer due to the chemical reaction in the stagnant film, then

$$q_{ch} = \left[2k_w T_e B \rho_w^2 Y_{O,e} Y_{F,e} \left(\frac{\theta_w^2}{E^*}\right) \alpha_{O,w} \alpha_{F,w}\right]^{1/2} e^{-E^*/2\theta_w} \qquad (105)$$

The convective surface heat transfer q_{con} is the next item to be considered. Sibulkin [54] obtained a solution for the convective heat transfer near the forward stagnation point of a blunt body of revolution. His results might be expressed in the form

$$Nu = 0.763\ Pr^{0.4} \sqrt{\frac{x}{u_\infty}\left[\frac{du_e}{dx}\right]_o} \sqrt{\frac{u_\infty x}{\gamma}} \qquad (106)$$

where x = distance along the surface measured for the stagnation point.

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u_∞ = gas stream approach velocity.

u_e = free-stream velocity outside the boundary layer.

$\left[\frac{du_e}{dx}\right]_o$ = free-stream velocity gradient at the stagnation point.

$$Nu = q_{con}x/k_w(T_w-T_e) \tag{107}$$

Equation (106) is valid for an incompressible flow with constant properties.

At the stagnation point

$$\left[\frac{du_e}{dx}\right]_o = a = u_e/x \tag{108}$$

Using equation (108), equation (106) reduces to

$$Nu = 0.763(Pr)^{0.4}\sqrt{(Re)_e} \tag{109}$$

where

$$(Re)_e = u_e x/\gamma_w \tag{110}$$

Thus the surface heat transfer due to convection alone is given by

$$q_{con} = 0.763k_w\left(\frac{1}{x}\right)(T_w-T_e)(Pr)^{0.4}\sqrt{(Re)_e} \tag{111}$$

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or
$$q_{con} = 0.763 k_w T_e \sqrt{\frac{a\rho_w}{\mu_w}} (\theta_w - 1)(Pr)^{0.4} \tag{112}$$

The Van't Hoff ignition criterion in this case can be written as

$$q_{ch} = q_{con} \tag{113}$$

Squaring and equating equations (105) and (112), they yield

$$2q^{o} B \rho_w \mu_w Y_{O,e} Y_{F,e} \theta_w^2 \alpha_{O,w} \alpha_{F,w} e^{-E^*/\theta_w} = k_w T_e E^* a(\theta_w - 1)^2 (Pr)^{0.8} \tag{114}$$

Before proceeding to transform equation (114) into a more suitable form, we will attempt to express the unknown quantities $\alpha_{O,w}$ and $\alpha_{F,w}$ in terms of known properties of the system. Combining equations (83) and (84) we have

$$\frac{d}{dy}\left[\rho D \frac{d}{dy}\left(\alpha_F/(\gamma_F W_F Y_{O,e}) - \alpha_O/(\gamma_O W_O Y_{F,e})\right)\right] = 0 \tag{115}$$

The solution of the above equation subject to the boundary conditions (98.b) and (99.b) is

$$\alpha_O = 1 - (1+\alpha_F)/(n_e+1) \tag{116}$$

where n_e is defined by equation (52).

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Generally speaking, the ignition condition, equation (113) can be written as

$$\partial T/\partial \hat{n} = 0 \tag{117}$$

In such a case (see page 88), the fuel mass fraction and the temperature are related by equation (90).

Thus using equations (116) and (90) and the definitions of the First and Second Damköhler numbers, equation (114) may be expressed in the form

$$\bar{D}_{I,i} = 0.145 \frac{E^*(\theta_w-1)^2 \bar{D}_{II}(Pr)^{0.2}}{\theta_w(1-\theta_w+\bar{D}_{II})^2} e^{E^*/\theta_w} \tag{118}$$

Equation (118) expresses the maximum value of the First Damköhler number $\bar{D}_I$ to secure ignition, in terms of the surface temperature of the heated body and other similarity parameters of the flow.

Figure 21 shows a plot of the First Damköhler number $\bar{D}_I$ versus the ignition temperature, θ_w, obtained from equation (118). For comparison, the corresponding curve obtained by the "exact method" was superimposed. It is evident that the approximate method gives excellent results for ignition temperatures up to $\theta_w = 5$. At higher wall temperatures the correlation does not hold. A possible explanation for the large differences obtained at high temperatures is that the convective heat transfer correlation used was obtained for the case of a frozen flow. Thus, as the state of the mixture departs from the frozen limit

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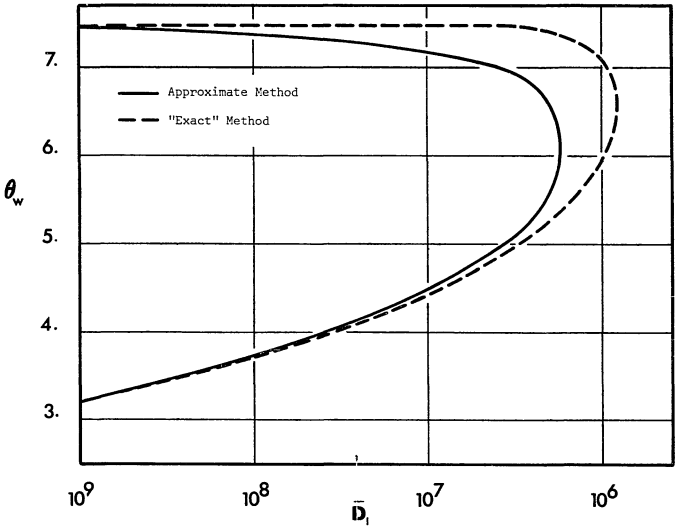

Figure 21. Ignition Temperature Versus D_I--Comparison of the Approximate and "Exact" Methods

towards the equilibrium limit, equation (118) becomes a crude approximation.

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CHAPTER VI

CONCLUSIONS

A theoretical study of the steady-state theory of ignition of a premixed combustible gas by a heated surface has been made. Based on similarity analysis, a general ignition equation was developed which relates the ignition temperature (surface temperature of the heated body) to appropriate dimensionless parameters of the reactive flow. Of these parameters, two are of primary importance in describing the ignition characteristics of the system: a) the First Damköhler number $\bar{D}_I$ which represents a measure of the residence time of a fluid particle in the reaction region relative to the chemical time, and b) the Nusselt number Nu which represents the magnitude of the heat transfer at the gas-solid interface.

As a specific example, the ignition of a gaseous combustible mixture in the stagnation region of a blunt body was considered. Under suitable assumptions the resulting differential equations governing the flow, were numerically integrated for a range of values of the First Damköhler number corresponding to the transition from frozen to equilibrium state.

From the Nusselt number-First Damköhler number relationship (Figure 3), two critical parameters were defined: the Ignition First Damköhler number, $\bar{D}_{I,i}$, and the Extinction First Damköhler number, $\bar{D}_{I,e}$. In the case of $\bar{D}_I > \bar{D}_{I,i}$ the flow is always in equilibrium.

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Similarly for $\bar{D}_I < \bar{D}_{I,e}$ the flow is always "frozen." In the central region defined by $\bar{D}_{I,e} \leq \bar{D}_I \leq \bar{D}_{I,i}$ the state of the mixture can lie on one of three branches:

i. the frozen branch A,

ii. the equilibrium branch C,

iii. an intermediate branch B which is unstable.

For a given surface temperature of the body, ignition of the combustible mixture will occur at $\bar{D}_I = \bar{D}_{I,i}$. The ignition process can be represented by the transition in the state of the mixture from branch A to branch C (see Figure 3) in accord with the transient nature of such processes. Likewise, extinction will occur at $\bar{D}_I = \bar{D}_{I,e}$. The extinction process can be represented by the transition from branch C to branch A.

The ignition of a premixed gaseous mixture in the stagnation region of a blunt body was also examined using the Van't Hoff criterion. This condition ($\partial T/\partial \hat{n}=0$) was introduced into the mathematical formulation of the problem as an additional boundary condition. For a given value of the First Damköhler number the ignition temperature θ_w was obtained by numerically solving the governing equations. A comparison with the results obtained using the surface heat transfer-First Damköhler number relation showed good agreement. Use of the Van't Hoff ignition criterion yields values of the ignition temperature slightly below those obtained by the former method. The discrepancy between the two methods increases with decreasing values of the First Damköhler number.

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The following are the results obtained on the effects of the free-stream velocity, free-stream temperature, inert gas concentration and activation energy on the ignition temperature.

1. Higher free-stream velocities require higher ignition temperatures. However, an upper limit on the velocity exists, beyond which ignition cannot occur.

2. Higher free-stream temperatures of the mixture facilitate ignition.

3. The presence of inert gases in the combustible mixture impedes ignition.

4. Lower activation energies of the reactants require lower ignition temperatures.

The above theoretical results are in accord with the experimental findings of Silver [12], Paterson [13,14] and Mullen [15].

An expression relating the Ignition First Damköhler number ($\bar{D}_{I,1}$) to the surface temperature of the heated body was obtained using a simplified analytical model. In this model, assuming that the gases near the surface of the heated body are at rest, the surface heat transfer due to the chemical reaction is equated to the convecting heat transfer of the corresponding frozen flow. This approach is similar to the thermal theory of ignition of Khitrin and Goldenberg [17]. A comparison of the "exact" method (solving the differential equations with the Van't Hoff criterion as a boundary condition) and the simplified method, showed close agreement for ignition temperature up to $\theta_w = 5$.

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The agreement of the results obtained by the above simplified method is of considerable importance in obtaining the ignition temperature of systems with complex flow patterns. In such systems, a complete solution of the governing equations is not practical. In order to obtain a relation similar to equation (118) for such flows, an expression of the frozen convective heat transfer coefficient is required. This can be obtained from past literature or through experimentation.

In conclusion, it must be noted that the above discussed steady-state approaches to the ignition of premixed gaseous mixtures by heated bodies do not indicate a minimum surface temperature of the body, below which no ignition is possible. However, at low surface temperatures of the body the corresponding values of the free stream velocity are so low that an infinite amount of time is required for a gas particle in the free-stream region to reach the surface of the body. Thus for such surface temperatures, the mixture will not ignite.

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