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EXACT AND APPROXIMATE SOLUTIONS OF A CHEMICALLY REACTING NONEQUILIBRIUM FLOW PROBLEM

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Abstract – By studying a two-dimensional flow problem, the consequences of employing approximation methods in ignition problems are elucidated. Asymptotic and local similarity solutions are obtained for flows over an adiabatic plate and over a perfectly conducting plate. The governing partial differential equations are transformed into a single integral equation in Von Mises space which is amenable to solutions by the Laplace method and by the assumption of a slowly varying function. To apply the technique of local similarity to the present problem, the usual boundary layer similarity transformation is used. The results are compared with an available exact numerical solution.

NOMENCLATURE

$\bar{a}$,	constants of integration in equation (23);
B,	dimensionless heat release parameter defined in equation (30);
$C_i, i=1,3$,	mass fraction of ith species;
C_{p_i},	specific heat of ith species;
$\bar{C}_p$,	average specific heat of gaseous mixture;
D,	diffusion coefficient of gaseous mixture;
E,	activation energy;
f,	reduced stream function defined in equation (36);
$f''(0)$,	$0.322\sqrt{2}$;
h_i,	enthalpy of ith species;
h,	enthalpy of gaseous mixture;
h_i^0,	heat of formation of ith species;
Δh^0,	heat of reaction defined in equation (27);
H,	non-dimensionalized enthalpy defined in equation (11);
J_{iw},	surface production rate of ith species;
J_w,	surface production rate defined in equation (10);
k,	frequency factor;
l,	$(\rho\mu)/(\rho\mu)_\infty$;
L,	length of plate;
Le,	Lewis number;
M_i,	molecular weight ith species;
$\bar{M}$,	average molecular weight of gaseous mixture;
p,	flow pressure;
Pr,	Prandtl number;
r,	parameter defined in equation (30);
R_g,	gas constant;
s,	space variable on Laplace transformed plane;
Sc,	Schmidt number;
T,	temperature;
T^0,	reference temperature;
u,	flow velocity in x-direction;
v,	flow velocity in y-direction;
W,	dimensionless consumption parameter defined in equation (16);
x,	distance along direction of gas flow;
x_T,	parameter defined by equation (30);
y,	coordinate normal to flow direction;
z,	transient space variable defined by equation (15);
α,	thermal diffusivity;
β,	dimensionless activation energy parameter defined in equation (19);
Δ,	shear stress defined by equation (20);
η,	similarity variable defined by equation (33);
θ,	non-dimensionalized temperature;
λ,	thermal conductivity;
μ,	dynamic viscosity;
ν'',	parameter defined in equation (44);
ξ,	dimensionless space variable defined in equation (33);
ρ,	density;
ϕ,	conversion defined in equation (11);
$\bar{\phi}$,	conversion in transformed plane;
ψ,	stream function.

Subscripts

0,	initial;
1,	CO;
2,	O_2;
3,	CO_2;
∞,	undisturbed region;
w,	wall.

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INTRODUCTION

THE INTERESTING aspects of nonequilibrium, chemically reacting boundary layers that originate from the interaction between the boundary-layer characteristics and the finite-rate chemical reactions are contained within a set of coupled nonlinear partial differential equations that describe the conservation of mass, energy, and momentum. In the case of surface, chemical reactions, these governing equations are identical to those for inert boundary layers. The chemical reaction effects on these equations enter through their boundary conditions. In certain situations, the corresponding chemically inert problems possess similarity solutions, whereas, in other instances, approximate solutions can sometimes be obtained through the so-called local similarity and local nonsimilarity methods. In the equilibrium limit, where the chemical reaction takes place at an infinitely fast rate as compared to the characteristic residence times of the chemical species, these existing solutions can be used, provided properly modified energy-driving potentials are defined. For the nonequilibrium case, where the chemical reaction proceeds at a finite rate, no such direct extension exists. In their desire to utilize directly the abundantly available chemically inert results, many researchers have either formulated approximate models or have resorted to certain approximation techniques of solutions of the equations. Several authors have adopted the local similarity assumption in their solutions, which has sometimes resulted in nonunique, multiple solutions for the steady state problems, even though the exact procedure leads to unique solutions. One of the objectives of the present work is to shed some light on the use and the consequences of these approximation methods and to elucidate the nature of the fallacious implications introduced by such methods of solutions.

Surface reactions can generally be classified in two categories. The surface either participates in the chemical reaction or may only act as a catalyst. The subjects of ignition and combustion of the solid fuel fall into the first category, and the problems of catalytic surface recombination of dissociated species and numerous other catalytic problems comprise the second. Liu [1] studied the transient problem of the onset of surface combustion in a still atmosphere. He concluded that the system could stabilize in either a weak or a diffusion-limited reaction mode. Waldman [2] questioned the validity of these inferences and showed that only a strong combustion mode is possible. Approximative analyses performed in his paper pointed to the possibility of three combustion states, which was declared to be physically implausible. Yung and Chung [3] correctly attributed the redundant combustion modes to the local similarity assumption, which is based on the qualitative notion that the ratio of time derivative to the function itself should be small. The correct solution, on the other hand, showed that the timewise temperature gradient at the incipient ignition point was so large that a term, 'thermal shock', was coined to explain its existence. The multiplicity arising in this situation can be quite simply discarded once it is realized that time cannot go backwards.

Another related study that merits a mention is due to Kashiwagi *et al.* [4]. Frustrated by the limitation of one-dimensional models in distinguishing the dominant ignition mechanism between surface and gas phase reaction theories for solid propellants, the authors resorted to a two-dimensional unsteady forced convective model. This model includes the surface regression of the solid surface and more importantly accounts for heat conduction in the transverse direction in the solid fuel of semi-infinite extent, thereby introducing time as an independent variable. The gas phase was considered to be in quasi-steady state. In order to reduce the complexity of the numerical computations, the local similarity approximation was invoked. The solution did not show any multiplicity; the results of the present study will help forward some explanations concerning this aspect of the solution.

Artyukh *et al.* [5] used the local similarity approach in deducing the ignition and extinction criteria associated with surface reactions. Lindberg and Schmitz [6] have shown that the extinction phenomenon they observed has no counterpart in the exact solution of the problem. During the numerical simulation, they found that multi-valued solutions are obtained when the increments in the longitudinal direction are not sufficiently small. Instead of directly integrating the governing equations, Mihail and Teodorescu [7] have numerically solved the superposition integral derived previously by Lighthill [8], Chambre [9], and others. With this approach, uniqueness of steady states was obtained independently of the step size. Lindberg and Schmitz also showed that the same boundary layer problem on a perfectly conducting solid plate admits genuine multiple solutions.

This work will apply analytical tools to the Lindberg and Schmitz problem of surface ignition in a flow system. The solid surface will be considered to be either adiabatic or perfectly conducting. In the latter case, solution will be obtained by the local similarity method. By comparison with an exact solution, it will be demonstrated that the local similarity approximation is valid in this case. For an adiabatic surface, solutions will be obtained by an asymptotic method and by the local similarity method. Although the former approach predicts unique solutions, the local similarity method produces multi-valued results. A comparison with an exact numerical solution will prove that the adiabatic surface ignition problem does not admit nonunique solutions. The accuracy of the asymptotic technique will be evaluated. The closed-form local similarity solutions will be obtained for subsequent comparison with correct solutions, by transforming the governing equations into equations in the similarity space. In order to furnish correct, although approximate, asymptotic solutions, the governing equations will be cast into an integral form. This can be done only by suitably approximating the velocity profile near the surface. Instead of producing the Lighthill type of integral equation, a nonlinear Volterra equation will be generated, which will be solved by employing the Laplace method of evaluating integrals in the case of an adiabatic plate. The essentially closed-form nature of the solutions will aid in deciphering correctly the characteristics of the approximation methods of solution.

DESCRIPTION OF THE PROBLEM

The model being considered is a two-dimensional system in which a stream of reactants flows past a solid surface. An exothermic reaction occurs on the solid surface. The solid may be either chemically reactive or merely catalytic in nature. Two kinds of thermal conditions at the solid surface are represented. In the first, the thermal conductivity of the solid is taken to be infinite. In the second case, the solid is very thin or its thermal conductivity is negligible, so that the boundary condition of an adiabatic surface is implied.

MATHEMATICAL FORMULATION

The following are the material, momentum, and energy boundary layer equations for flow past a flat plate that account for a finite-rate chemical reaction on a solid surface.

Continuity:

$$\frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) = 0. \tag{1}$$

Momentum:

$$\rho u\frac{\partial u}{\partial x} + \rho v\frac{\partial u}{\partial y} = \frac{\partial}{\partial y}\left(\mu\frac{\partial u}{\partial y}\right). \tag{2}$$

Conservation of energy:

$$\rho u\frac{\partial h}{\partial x} + \rho v\frac{\partial h}{\partial y} = \frac{\partial}{\partial y}\left(\frac{\mu}{Pr}\frac{\partial h}{\partial y}\right). \tag{3}$$

Conservation of species:

$$\rho u\frac{\partial C_i}{\partial x} + \rho v\frac{\partial C_i}{\partial y} = \frac{\partial}{\partial y}\left(\frac{\mu}{Sc}\frac{\partial C_i}{\partial y}\right). \tag{4}$$

Where

$$h = \Sigma C_i h_i,$$

$$h_i = h_i^0 + \int_{T^0}^{T} C_{p_i}\,\mathrm{d}T. \tag{5}$$

Initial conditions,

at $x = 0,\quad y \geq 0$:

$$u = u_\infty,\quad v = 0,\quad T = T_\infty,\quad C_i = C_{i\infty}.$$

Boundary conditions,

$$\text{at}\quad x > 0,\quad y = 0$$

$$u = v = 0$$

$$\rho D\frac{\partial C_i}{\partial y} = J_{iw}. \tag{6}$$

For perfectly conducting plate

$$\int_0^L \left(\frac{\partial h}{\partial y}\right)_{y=0} \mathrm{d}x = 0 \quad \text{and} \quad T_w = \text{const}. \tag{7}$$

For adiabatic plate,

$$\left(\frac{\partial h}{\partial y}\right)_{y=0} = 0.$$

At $\quad x > 0,\quad y \to \infty,$

$$u = u_\infty,\quad T = T_\infty,\quad C_i = C_{i\infty}.$$

Some of the assumptions adopted in this study are: the gaseous mixture behaves like a perfect gas whose Prandtl and Schmidt numbers are constant and equal; the specific heat of the gaseous mixture is a constant, and the ratio, $\rho\mu/\rho_\infty\mu_\infty$, is a constant, l. The gaseous mixture is considered to be frozen, and the pressure is taken as a constant. The energy equation can also be written in terms of temperature as

$$\rho u\frac{\partial T}{\partial x} + \rho v\frac{\partial T}{\partial y} = \frac{\partial}{\partial y}\left(\frac{\mu}{Pr}\frac{\partial T}{\partial y}\right). \tag{8}$$

In order to compare the results directly with those of Lindberg and Schmitz, the reaction model of those authors is used in this study. The kinetic model considered was the catalytic oxidation of carbon monoxide on a silver–palladium catalyst. Carbon monoxide (subscript 1) and oxygen (subscript 2) react irreversibly to form carbon dioxide (subscript 3) according to the following stoichiometry:

$$CO + \tfrac{1}{2}O_2 \rightarrow CO_2.$$

Thus,

$$\phi = \frac{C_{1\infty} - C_1}{C_{1\infty}} = \frac{2M_1}{M_2}\left(\frac{C_{2\infty} - C_2}{C_{1\infty}}\right) = -\frac{M_1}{M_3}\left(\frac{C_{3\infty} - C_3}{C_{1\infty}}\right) \tag{9}$$

where M denotes molecular weight. The rate expression was represented by the following second-order Arrhenius type relationship:

$$J_w = kT\rho^2 C_1 C_2 \exp\left(-\frac{E}{R_g T}\right). \tag{10}$$

The kinetic constants, E and k, were taken as 48.5 kJ/mol and 0.013 m^4/(s.kg.K), respectively. The additional data used in their calculations are given below:

$$p = 1\ \text{atm},\quad T_\infty = 473\ \text{K},\quad T^0 = 298\ \text{K},$$

$$(\rho\mu u)_\infty = (\rho^2 D)u_\infty = 7.98 \times 10^{-6}\ \text{kg}^2/(\text{m}^3\,\text{s}^2),$$

$$C_{1\infty} = 0.1,\quad C_{2\infty} = 0.9,\quad C_{3\infty} = 0,$$

$$h_1^0 = -3.95\ \text{kJ/g},\quad h_2^0 = -8.94\ \text{kJ/g},\quad h_3^0 = 0.$$

The following nondimensional variables are defined,

$$\theta = \frac{T - T_\infty}{T_\infty},\quad \phi = \frac{C_{i\infty} - C_i}{b_i C_{1\infty}},\quad H = \frac{h_\infty - h}{h_\infty}, \tag{11}$$

where b_i is the stoichiometric coefficient for component i and J_w is equal to J_{iw}/b_i.

First, the continuity equation is satisfied by defining the stream function, ψ, in the standard manner [10] (i.e. $\partial\psi/\partial x = -\rho v$, $\partial\psi/\partial y = \rho u$). Solution of the momentum equation, equation (2), is well known. Utilizing the surface shear stress, $\Delta(x)$, available from the solution, the velocity, u, is replaced by its assymptotic form near the surface, after Fage and Falkner [11].

This is acceptable because it is the velocity profile near the surface that most influences the temperature and the distribution of chemical species. Thus,

$$u = \frac{\Delta(x)}{\mu_w} y, \tag{12}$$

where $\Delta(x)$ is the shear stress at the wall. The stream function, ψ, can now be approximated as,

$$\psi = \int_0^y \rho u \, \mathrm{d}y \sim \int_0^y (\rho\mu)_w \frac{\mathrm{d}u}{\Delta(x)} = \frac{1}{2} \frac{(\rho\mu)_w}{\Delta(x)} u^2,$$

which relates u with ψ in the following way:

$$u = \left(\frac{2\Delta(x)}{\rho_w \mu_w}\right)^{1/2} \psi^{1/2}. \tag{13}$$

The governing equations, when transformed from (x, y) to (z, ψ) plane, are:

$$\frac{\partial Y}{\partial z} = \frac{\partial}{\partial \psi}\left(\psi^{1/2} \frac{\partial Y}{\partial \psi}\right), \tag{14}$$

where Y may represent θ, H, or ϕ, and z is a transient independent variable defined as,

$$z = \frac{1}{Pr} \int_0^x [2l(\rho\mu)_\infty \Delta(x)]^{1/2} \, \mathrm{d}x. \tag{15}$$

The transformed initial and boundary conditions are:

$$\theta(0, \psi) = \phi(0, \psi) = H(0, \psi) = 0,$$

$$\left(\psi^{1/2} \frac{\partial \phi}{\partial \psi}\right)_{\psi=0} = -\frac{Pr}{C_{1\infty}} \frac{J_w}{\sqrt{[2l(\rho\mu)_\infty \Delta(z)]}} = \tfrac{1}{2} W(z), \tag{16}$$

$$\left.\begin{aligned} &\int_0^{z_L} \left(\psi^{1/2} \frac{\partial H}{\partial \psi}\right)_{\psi=0} \mathrm{d}z = 0 \quad \text{for a perfectly conducting plate,} \\ &\left(\psi^{1/2} \frac{\partial H}{\partial \psi}\right)_{\psi=0} = 0 \quad \text{for an adiabatic plate} \end{aligned}\right. \tag{17}$$

where

$$J_w = k\rho_\infty^2 C_{1\infty} C_{2\infty} T_\infty \frac{\mathrm{e}^{-\beta}}{(1+\theta_w)} \exp\left(\frac{\beta\theta_w}{1+\theta_w}\right) \times (1-\phi_w)\left(1 - \frac{M_2}{2M_1} \frac{C_{1\infty}}{C_{2\infty}} \phi_w\right) \tag{18}$$

and

$$\beta = \frac{E}{R_g T_\infty}. \tag{19}$$

The shear stress, $\Delta(x)$, is given by the following equation:

$$\Delta(x) = \left(\mu \frac{\partial u}{\partial y}\right)_w = \left(\frac{(\rho\mu)_\infty l}{2u_\infty x}\right)^{1/2} f''(0) u_\infty^2 \tag{20}$$

where $f''(0)$ is the Blasius surface shear available as the solution of equation (2). With the use of the above representation for $\Delta(x)$, equation (15) becomes

$$z = \frac{2}{3} \frac{[2f''(0)]^{1/2}}{Pr} (2l(\rho\mu u)_\infty)^{3/4} x^{3/4}. \tag{21}$$

ANALYSIS

The governing partial differential equations for the adiabatic plate and for the perfectly conducting plate will now be analyzed by an asymptotic technique and by a local similarity method. In order to apply the asymptotic technique, the reactant conversion equation in the (z, ψ) plane is first transformed into a nonlinear integral equation, subsequently simplified for the case of adiabatic plate by the Laplace method of evaluating integrals with a large parameter. For the purpose of obtaining local similarity solutions, the governing equations are transformed into a similarity space. True similarity solutions are possible only in the frozen and equilibrium limits. In the context of local similitude, however, non-similar terms consisting of longitudinal derivatives are dropped and the axial variable is treated as a parameter. The analytic results from the two methods will be compared with an exact numerical solution.

1. *Solution by asymptotic method*

(a) *Adiabatic plate.* The linear governing equations, (14), are transformed in the independent variable z as follows:

$$\frac{\mathrm{d}}{\mathrm{d}\psi}\left(\psi^{1/2} \frac{\mathrm{d}\bar{Y}}{\mathrm{d}\psi}\right) - s\bar{Y} = 0 \tag{22}$$

where $\bar{Y}$ is the Laplace transform defined as

$$\bar{Y} = \int_0^\infty \mathrm{e}^{-sz} Y(z, \psi) \mathrm{d}z.$$

The solution of equation (22), which is finite in the limit of $\psi \to \infty$, is

$$\bar{Y} = \bar{a}\psi^{1/4} K_{1/3}\left(\frac{4}{3}\sqrt{s}\,\psi^{3/4}\right) \tag{23}$$

where $K_{1/3}$ is the one-third order modified Bessel function of the second kind. On applying the boundary condition given by equation (16), the following equation results for $\bar{\phi}_w$:

$$\bar{\phi}_w = -\left(\frac{3}{2}\right)^{2/3} \frac{\Gamma(4/3)}{\Gamma(2/3)} \frac{\bar{W}(s)}{s^{1/3}} \tag{24}$$

Using the convolution theorem, the inverse transformation of the above equation is

$$\bar{\phi}_w = -\left(\frac{3}{2}\right)^{2/3} \frac{\Gamma(4/3)}{\Gamma(2/3)} \int_0^z W(z')$$

$$\times \frac{1}{(z-z')^{2/3}} \frac{1}{\Gamma(1/3)} \mathrm{d}z'. \quad (25)$$

On employing the enthalpy and conversion defining equations, (5) and (11), H can be expressed as

$$H = 1 - \frac{1}{h_\infty}[C_{1\infty}h_1^0 + C_{2\infty}h_2^0 + C_{3\infty}h_3^0 + \bar{C}_p(T-T^0) - \phi\,\Delta h^0 C_{1\infty}] \quad (26)$$

where

$$\Delta h^0 = h_1^0 + \frac{M_2}{2M_1}h_2^0 - \frac{M_3}{M_1}h_3^0. \quad (27)$$

For the adiabatic plate, solution of the energy equation, expressed in terms of the enthalpy function H, is trivially obtained as

$$H = 0,$$

so that, with the help of equation (26),

$$\phi = \left(\frac{\bar{C}_p T_\infty}{C_{1\infty}\Delta h^0}\right)\theta. \quad (28)$$

With the availability of the above relationship, it is necessary only to solve the ϕ equation, (25), to describe the flow system. After some mathematical manipulation of equation (25), the following integral equation obtains:

$$\theta_w = \frac{1}{\sqrt{2}}\left(\frac{4}{3}\right)^{2/3} \frac{1}{\Gamma(2/3)} \times \frac{Pr^{2/3}k\rho_\infty^2 T_\infty C_{2\infty}\,\mathrm{e}^{-\beta}}{(l(\rho\mu u)_\infty)^{1/2}[f''(0)]^{1/3}}\left(\frac{C_{1\infty}\Delta h^0}{\bar{C}_p T_\infty}\right) \times \int_0^{x_T} \frac{1}{(1+\theta_w)}\left(1-\frac{\theta_w}{B}\right)\left(1-\frac{\theta_w}{rB}\right) \times \exp\left(\frac{\beta\theta_w}{1+\theta_w}\right)\frac{x'^{1/3}}{(x_T-x')^{2/3}}\,\mathrm{d}x' \quad (29)$$

where

$$B = \frac{C_{1\infty}\Delta h^0}{\bar{C}_p T_\infty}, \qquad r = \frac{2M_1}{M_2}\frac{C_{2\infty}}{C_{1\infty}},$$

and (30)

$$x_T = x^{3/4}.$$

From physical reasoning, the surface temperature for an adiabatic plate is a monotonically increasing function of x, so that the Laplace method may be employed to evaluate the integral in equation (29) asymptotically as follows [12, 13]:

$$\int_0^{x_T} \frac{x'^{1/3}}{(1+\theta_w)}\left(1-\frac{\theta_w}{B}\right)\left(1-\frac{\theta_w}{rB}\right) \times \exp\left(\frac{\beta\theta_w}{1+\theta_w}\right)\frac{\mathrm{d}x'}{(x_T-x')^{2/3}}$$

$$\simeq \frac{x_T^{1/3}}{(1+\theta_w)}\left(1-\frac{\theta_w}{B}\right)\left(1-\frac{\theta_w}{rB}\right)\exp\left(\frac{\beta\theta_w}{1+\theta_w}\right)\int_0^{x_T} \exp\left\{\left[\frac{\beta}{(1+\theta_w)^2}\left.\frac{\mathrm{d}\theta_w}{\mathrm{d}x'}\right|_{x'=x_T}\right](x'-x_T)\right\} \times \frac{\mathrm{d}x'}{(x_T-x')^{2/3}}$$

$$= \frac{x_T^{1/3}}{(1+\theta_w)}\left(1-\frac{\theta_w}{B}\right)\left(1-\frac{\theta_w}{rB}\right) \times \exp\left(\frac{\beta\theta_w}{1+\theta_w}\right)\left[\frac{(1+\theta_w)^2}{\beta(\mathrm{d}\theta_w/\mathrm{d}x_T)}\right]^{1/3} \times \lim_{\beta\to\infty}\int_0^{\left[\frac{\beta(\mathrm{d}\theta_w/\mathrm{d}x_T)}{(1+\theta_w)^2}\right]x_T} \mathrm{e}^{-x_1}x_1^{-2/3}\,\mathrm{d}x_1$$

$$\simeq \frac{x_T^{1/3}}{(1+\theta_w)}\left(1-\frac{\theta_w}{B}\right)\left(1-\frac{\theta_w}{rB}\right)\exp\left(\frac{\beta\theta_w}{1+\theta_w}\right) \times \left[\frac{(1+\theta_w)^2}{\beta(\mathrm{d}\theta_w/\mathrm{d}x_T)}\right]^{1/3}\int_0^\infty \mathrm{e}^{-x_1}x_1^{-2/3}\,\mathrm{d}x_1$$

$$= \Gamma(1/3)\frac{x_T^{1/3}}{(1+\theta_w)}\left(1-\frac{\theta_w}{B}\right)\left(1-\frac{\theta_w}{rB}\right) \times \exp\left(\frac{\beta\theta_w}{1+\theta_w}\right)\left[\frac{(1+\theta_w)^2}{\beta(\mathrm{d}\theta_w/\mathrm{d}x_T)}\right]^{1/3}. \quad (31)$$

Finally, on rearrangement:

$$\theta_w^3\frac{\mathrm{d}\theta_w}{\mathrm{d}x} = \frac{1}{\beta}\left[\frac{\sqrt{3}}{2\sqrt{2\pi}}\left(\frac{4}{3}\right)^{1/3} \times \frac{[\Gamma(1/3)]^2 Pr^{2/3}k\rho_\infty^2 T_\infty C_{2\infty}\,\mathrm{e}^{-\beta}}{[l(\rho\mu u)_\infty]^{1/2}[f''(0)]^{1/3}}B\right]^3 \times \frac{x^{1/2}}{(1+\theta_w)}\left(1-\frac{\theta_w}{B}\right)^3 \times \left(1-\frac{\theta_w}{rB}\right)^3\exp\left(\frac{3\beta\theta_w}{1+\theta_w}\right). \quad (32)$$

The numerical computation involved in integrating equation (32) is almost trivial compared with solving equation (25), from which it was derived.

(b) *Perfectly conducting plate.* In the case of the perfectly conducting plate, the surface acquires a uniform temperature. In this situation, the Arrhenius term of the chemical reaction term [W(z')] in equation (5) loses its positional dependence and becomes a constant above z'. This leads to the hypothesis that $W(z')$ is a slowly varying function in comparison with the term $1/(z-z')^{2/3}$, which has a removable singularity at the upper limit of the integral under consideration. But this is, indeed, the premise upon which the local similarity method is based, and the corresponding term in that method is much easier to handle. For that reason, this approach for the perfectly conducting plate is abandoned here in favor of the local similarity method.

2. *Solution by local similarity method*

(a) *Perfectly conducting plate.* For analysis of problems by the local similarity method, it is convenient to transform the parabolic equations into a similarity space, which reveals the true nature of the parabolic problem. The following similarity variables are defined:

$$\xi = \int_0^x (\rho\mu u)_\infty \mathrm{d}x = (\rho\mu u)_\infty x,$$

$$\eta = \frac{(\rho\mu)_\infty}{\sqrt{(2l\xi)}} \int_0^y \frac{\rho}{\rho_\infty}\mathrm{d}y. \tag{33}$$

The transformed governing equations are

$$f''' + ff'' = 0. \tag{34}$$

and

$$\frac{1}{Pr}Y'' + fY' = 2\xi f'\frac{\partial Y}{\partial \xi} \tag{35}$$

where f is the nondimensional stream function,

$$f = \frac{\psi}{\sqrt{(2l\xi)}}, \tag{36}$$

and the prime denotes differentiation with respect to η. The transformed initial and boundary conditions are:

at $\quad \xi = 0, \quad \eta > 0,$

$\quad f = f' = 0, \quad \theta = 0, \quad \phi = 0,$

at $\quad \xi > 0, \quad \eta = 0,$

$\quad f = f' = 0,$

$$\frac{\partial \phi}{\partial \eta} = -\left(\frac{2\xi}{l}\right)^{1/2}\frac{Sc}{(\rho\mu u)_\infty C_{1\infty}} J_w, \tag{37}$$

$$\int_0^{\xi_L} \frac{1}{\sqrt{\xi}}\left(\frac{\partial H}{\partial \eta}\right)_{\eta=0}\mathrm{d}\xi = 0. \tag{38}$$

The local similarity method is founded on the notion that changes in the streamline direction (ξ) are sufficiently small that the streamwise derivatives in equation (35) may be neglected. The variable ξ appears explicitly only through the boundary conditions. The velocity approximation of equation (12) gives for $f(\eta)$

$$f = f''(0)\eta^2/2 \tag{39}$$

where $f''(0)$ is obtained from the existing exact solution of the momentum equation (34). The solution of the remaining equation (35) is

$$\phi = \left(\frac{2}{l}\right)^{1/2}\frac{Sc}{(\rho\mu u)_\infty C_{1\infty}}\xi^{1/2} J_w \int_\eta^\infty \times \exp\left(-\frac{f''(0)Sc\,\eta^3}{6}\right)\mathrm{d}\eta$$

and $\qquad (40)$

$$\theta = \theta_w\left[1 - \left(\frac{9}{2}\right)^{1/3}\frac{[f''(0)Pr]^{1/3}}{\Gamma(1/3)}\int_0^\eta \times \exp\left(-\frac{f''(0)Pr\,\eta^3}{6}\right)\mathrm{d}\eta\right],$$

so that

$$\phi_w = \frac{1}{\sqrt{2}}\left(\frac{4}{3}\right)^{2/3}\Gamma\left(\frac{1}{3}\right)\frac{Pr^{2/3}k\rho_\infty^2 T_\infty C_{2\infty}\mathrm{e}^{-\beta}}{[l(\rho\mu u)_\infty]^{1/2}[f''(0)]^{1/3}} \times \frac{\exp\left(\dfrac{\beta\theta_w}{1+\theta_w}\right)}{(1+\theta_w)}(1-\phi_w)(1-r\phi_w)x^{1/2}, \tag{41}$$

and

$$\left(\frac{\partial\theta}{\partial\eta}\right)_{\eta=0} = -\left(\frac{9}{2}\right)^{1/3}\frac{Pr^{1/3}[f''(0)]^{1/3}}{\Gamma(1/3)}\theta_w. \tag{42}$$

Substituting equations (37) and (42) into (38), and making use of equation (41) yields:

$$\begin{aligned}
&(1+r) + r\left(\frac{v''}{\sqrt{L}}\right) - \left[(r-1)^2 + 2r(1+r)\left(\frac{v''}{\sqrt{L}}\right) + r^2\left(\frac{v''}{\sqrt{L}}\right)^2\right]^{1/2} - \frac{r(1+r)}{(r-1)}\left(\frac{v''}{\sqrt{L}}\right)\\
&\times \ln\left\{\frac{(r-1)\left[(r-1)^2 + 2r(1+r)\left(\frac{v''}{\sqrt{L}}\right) + r^2\left(\frac{v''}{\sqrt{L}}\right)^2\right]^{1/2} + (r-1)^2 + r(1+r)\left(\frac{v''}{\sqrt{L}}\right)}{2r^2\left(\frac{v''}{\sqrt{L}}\right)}\right\}\\
&+ r\left(\frac{v''}{\sqrt{L}}\right)\ln\left\{\frac{\left[(r-1)^2 + 2r(1+r)\left(\frac{v''}{\sqrt{L}}\right) + r^2\left(\frac{v''}{\sqrt{L}}\right)^2\right]^{1/2} + (r+1) + r\left(\frac{v''}{\sqrt{L}}\right)}{2r\left(\frac{v''}{\sqrt{L}}\right)}\right\}
\end{aligned} \tag{43}$$

$$= 2\left(\frac{\bar{C}_p T_\infty}{C_{1\infty}\Delta h^0}\right)\theta_w,$$

where

$$v'' = \sqrt{2}\left(\frac{3}{4}\right)^{2/3}\frac{1}{\Gamma(1/3)} \times \frac{[l(\rho\mu u)_\infty]^{1/2}[f''(0)]^{1/3}}{Pr^{2/3}k\rho_\infty^2 T_\infty C_{2\infty}\mathrm{e}^{-\beta}}\cdot\frac{(1+\theta_w)}{\exp\left(\dfrac{\beta\theta_w}{1+\theta_w}\right)}. \tag{44}$$

Before these solutions are discussed, the adiabatic case will be analyzed by the local similarity method also.

(b) *Adiabatic plate.* Equation (41), derived earlier for the case of perfectly conducting plate, is equally valid here. With the help of the relationship between the fractional conversion and the nondimensional temperature given by equation (28), (41) may be modified to yield the following algebraic equation:

$$\theta_w = \frac{1}{\sqrt{2}}\left[\left(\frac{4}{3}\right)^{2/3}\Gamma(1/3)\frac{Pr^{2/3}k\rho_\infty^2 T_\infty C_{2\infty}\, e^{-\beta}}{[l(\rho\mu u)_\infty]^{1/2}[f''(0)]^{1/3}}B\right]$$

$$\times\left(1-\frac{\theta_w}{B}\right)\left(1-\frac{\theta_w}{rB}\right)\frac{\exp\left(\dfrac{\beta\theta_w}{1+\theta_w}\right)}{(1+\theta_w)}x^{1/2}. \quad (45)$$

In all numerical computations, the parameters l, $\bar{C}_p$, and $\bar{M}$, the average molecular weight of the mixture were assigned values of 1, 0.53 kJ/($g \cdot k$) and 32 g/g · mole, in that order.

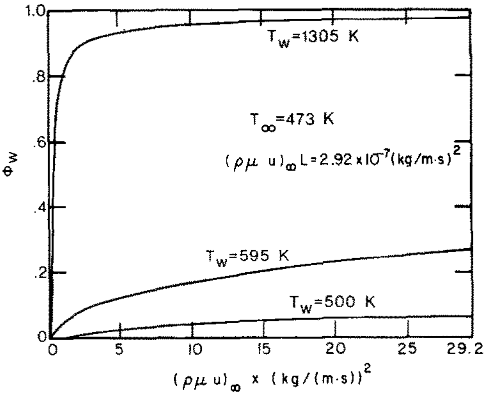

FIG. 2. Surface concentration profile for perfectly conducting plate.

RESULTS AND DISCUSSION

It should be noted that the temperature has a much greater influence on the reaction rate than does the concentration. For a perfectly conducting plate, the surface attains a uniform temperature, which induces the reaction rate to be a slowly varying function, and the integral equation degenerates into a nonlinear algebraic equation with possible multi-valued solutions associated with it. The same ignition behavior is also predicted by the exact numerical analysis. Van Heerden [14] states that a necessary condition for multiplicity in exothermic processes is a feedback of heat along the reaction path. The conduction of heat along the axial direction in the plate provides the necessary feedback in this case. As shown in Figs. 1 and 2, three combustion modes are possible. There are two stable solutions: at low temperature and low degree of conversion, and at high temperature and high degree of conversion. The middle combustion mode corresponds to an unstable ignition state. The two stable solutions represent the extinguished and fully-ignited states and are, respectively, chemically and diffusion controlled.

In the case of a perfectly conducting plate, θ_w is constant and equation (40) expresses a true similarity solution in which θ is a function of the similarity variable, η, only. For an adiabatic surface, on the other hand, θ_w as given by the implicit relationship of equation (45) leads to spurious multi-valued solutions not present in the exact solution of the governing equations. Figure 3 shows an interesting feature, namely, that according to the local similarity method, as the free stream temperature is increased, the region of multiplicity narrows and ultimately vanishes.

As explained by Kashiwagi *et al.* in [4], the adiabatic surface model of the present study may be regarded as a rough steady state analogue of their unsteady situation. Whereas both equation (45), based on local similarity method, and equation (32), based on physically correct Laplace asymptotic method, show x/u_∞ to be a naturally occurring parameter implying that the ignition delay distances should be proportional to free stream velocity, [4] found the first ignition point to be always near the leading edge. This discrepancy was attributed to the different boundary conditions considered in the steady state and unsteady state models. In the case of adiabatic surface, as considered in the present steady state model, the excess energy released by the surface reaction is stored entirely in the gas phase. However, in the unsteady state model, because initially the surface is cold, the excess energy goes into heating the solid phase so that the downstream part is too cold to initiate substantial chemical reaction. For this reason, ignition occurs at

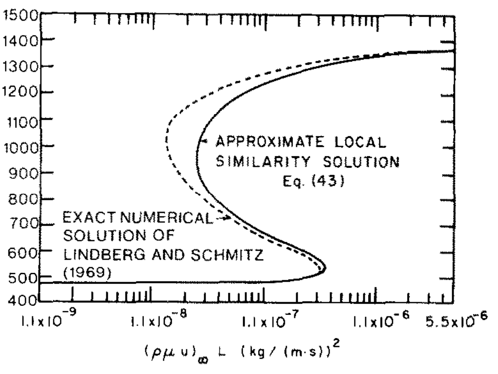

FIG. 1. Surface temperature dependence on plate length for perfectly conducting plate.

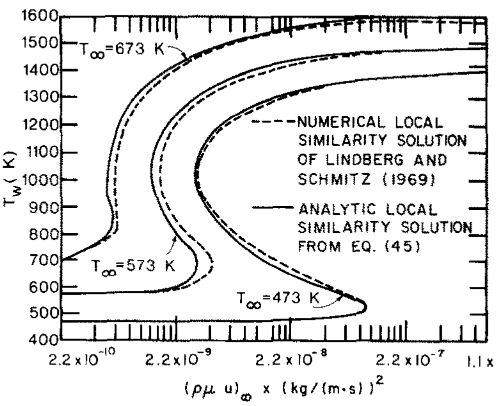

FIG. 3. Local similarity solutions for adiabatic plate.

the leading edge after a lapse of some time (ignition delay time) when the surface has become hot enough, and the first ignition point is always in a forward location. Subsequently, ignition commences at downstream positions and the steady state solution of the present study is approached asymptotically in time.

Figure 4 points to the extent of inaccuracy inherent in the use of local similarity method for an adiabatic surface. Kashiwagi *et al.* [4] also recognize this limitation and in a follow-up study [15] results were presented (for the gas phase ignition problem) without employing the local similarity assumption. The qualitative agreement in results of the two studies consolidate the conclusion that local similarity method when applied to the conducting-surface ignition problem produces results which are at least qualitatively correct. On physical grounds, the unsteady problem as formulated allows only transverse conduction of heat into the solid phase, hence there is no feedback along the streamwise direction. Therefore, no multiple solutions are expected to exist. Results of [4] do not indicate any spurious multiple solution being introduced by the local similarity method either. On the other hand, Fig. 3 has already confirmed that in the case of an adiabatic surface, the local similarity method leads to physically unrealistic multiple solutions. It is proposed that in the unsteady model, the extra mechanism of heat diffusion into the solid phase (as compared to the adiabatic surface) relieves the longitudinal gradient of surface temperature, thereby enabling the local similarity method to accommodate correctly the less abruptly changing character of the solution.

Figure 4 also provides a comparison between the results obtained by the present Laplace asymptotic method and the exact numerical solution of Lindberg and Schmitz. To make the problem amenable to closed-form solutions in the present work, three assumptions not previously used for finite difference solutions have been employed. The specific heat was regarded as constant, and the gas phase density assumed to be a function of the temperature only. An approximate velocity profile that is asymptotically correct at the solid surface has been used. In spite of these simplifications, the agreement between the results is excellent, even for a relatively low value of the nondimensional activation energy parameter, β. As opposed to the local similarity results, the solution changes abruptly from a kinetically controlled to a diffusion controlled regime near the ignition point.

It should be pointed out that the assumption of unity Lewis number can be readily relaxed by following the special technique developed in [16]. According to this method, equation (25) for reactant conversion and the like equation for temperature are to be handled separately. The two equations can be simplified by applying the Laplace method to them individually and then solved simultaneously. The full details of the procedure will be disclosed in a future publication.

The provision of feedback is not a necessary condition for existence of multiplicity. In a follow-up paper by Lindberg and Schmitz [17], involving flow past a blunt adiabatic object, the solution possessed genuine multiplicity. This was explained on the basis of possible multiple stagnation or 'initial' states. It should be mentioned in this connection that the existence of simple and multiple transitions between frozen and equilibrium limits in the case of gas phase diffusion flames for the stagnation mixing layer has also been studied extensively in the past [18]. The mixing layer is created by a jet of fuel meeting an oncoming stream of oxidant at the stagnation region of a blunt body. Stated simply, the multiplicity of states occurred when the nonlinearity in the reference Damkohler number became exceedingly large. For instance, a strong exothermic reaction can greatly increase the temperature of the reaction zone from the original value, without the reaction causing the exponential function of the local Damkohler number to vary by an order of magnitude. Lindberg and Schmitz refer to this as the possible source of multiple initial states. It follows that these authors would not have observed multiplicity had they considered an example wherein the kinetic rates were lower or the residence time was smaller. Finally, the stagnation point multiplicity is possible only because the local Damkohler number is independent of the longitudinal coordinate in the stagnation region.

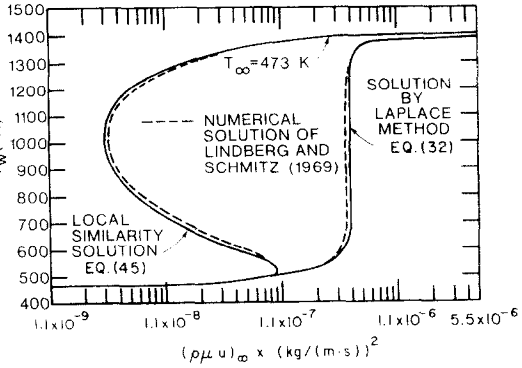

Fig. 4. Surface temperature profile for adiabatic plate.

CONCLUSIONS

A forced convective ignition problem has been analyzed. For the case of a perfectly conducting plate, the surface temperature is constant, and the local similarity hypothesis is physically applicable. Three combustion modes, two stable and one unstable are possible. For an adiabatic surface there is, near the ignition point, a sudden change in the character of the solution from a kinetically controlled to a diffusion controlled regime. Depending upon the free stream temperature and other flow conditions, the local similarity hypothesis may not accommodate the abruptness, and may produce multi-values results that are at variance with reality. The Laplace method of evaluating integrals is mathematically exact in the limit of β approaching infinity. The usefulness of the asymptotic technique can be judged from the fact that the results are in excellent agreement with the exact numerical solution, even though the value of the nondimensional activation energy parameter was only 12.34 and the velocity profile used in the computations was an approximation. It has been found that the ignition distance is proportional to the product of the free stream velocity and the inverse of the square of the oxidant concentration. This is in apparent conflict with the findings of a previous study on the determination of the dominant ignition mechanism in solid propellants; this discrepancy has been explained.

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SOLUTIONS EXACTE ET APPROCHEE D'UN PROBLEME D'ECOULEMENT AVEC REACTION CHIMIQUE HORS D'EQUILIBRE

Résumé — En étudiant un problème d'écoulement bidimensionnel, on dégage les conséquences de l'emploi de méthodes approchées dans les problèmes d'ignition. Des solutions asymptotiques et à similarité locale sont obtenues pour des écoulements sur une plaque adiabatique et sur une plaque parfaitement conductrice. Les équations aux dérivées partielles sont transformées dans l'espace de Von Mises en une seule équation intégrale qui est résolue par la méthode de Laplace et avec l'hypothèse d'une fonction lentement variable. Pour appliquer la technique de la similarité locale, on utilise la transformation classique pour la couche limite. Les résultats sont comparés à la solution numérique exacte.

EXAKTE UND ANGENÄHERTE LÖSUNGEN FÜR EIN STRÖMUNGSPROBLEM MIT CHEMISCHER REAKTION UND IM NICHTGLEICHGEWICHTSZUSTAND

Zusammenfassung—Anhand der Untersuchung eines zweidimensionalen Strömungsproblems werden die Folgen erläutert, die sich aus der Anwendung von Näherungsmethoden bei Zündungsproblemen ergeben. Für Strömungen über eine adiabate und über eine vollkommen leitende Platte werden asymptotische Lösungen und Lösungen örtlicher Ähnlichkeit erzielt. Die bestimmenden partiellen Differentialgleichungen werden in eine einzige Integralgleichung im von Mises-Raum transformiert, die sich mittels der Laplace-Methode und unter der Voraussetzung einer sich schwach ändernden Funktion lösen läßt. Um die Methode der örtlichen Ähnlichkeit auf das vorliegende Problem anwenden zu können, wird die übliche Grenzschicht-Ähnlichkeitstransformation angewandt. Die Ergebnisse werden mit einer vorliegenden exakten numerischen Lösung verglichen.

ТОЧНЫЕ И ПРИБЛИЖЕННЫЕ РЕШЕНИЯ ЗАДАЧИ О ХИМИЧЕСКИ РЕАГИРУЮЩЕМ НЕРАВНОВЕСНОМ ТЕЧЕНИИ

Аннотация — На основе изучения задачи о двумерном течении выяснена возможность использования приближенных методов для решения задач по воспламенению. Получены асимптотические и локально-подобные решения для случаев обтекания адиабатической и идеально проводящей пластин. Основные дифференциальные уравнения в частных производных преобразуются в одно интегральное уравнение в пространстве Мизеса, решение которого можно получить с помощью метода Лапласа и допущения о медленно изменяющейся функции. Для применения метода локального подобия используется обычное автомодельное преобразование пограничного слоя. Проведено сравнение результатов с имеющимся точным численным решением.