Nonadiabatic Propagation of a Planar Premixed Flame: Constant-Volume Enclosure

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The unsteady one-dimensional laminar nonisobaric propagation of a flame through a gaseous fuel-lean combustible premixture, characterized by large Arrhenius activation temperature, is examined under Shvab-Zeldovich-type formulation, via numerical integration by the method of lines with spline interpolation. The premixture is confined between plane parallel impervious noncatalytic isothermal walls, although adiabatic walls are also considered. The straightforward extension of the Shvab-Zeldovich approximation adopted is suppression of acoustic phenomena, nonessential for present purposes, by taking the pressure to be temporally variant, but spatially uniform. The relative importance of three phenomena not present in isobaric flame propagation (the variation of the diffusion coefficient with pressure, the change of the reaction rate with pressure, and the explicit temporal-pressure-derivative contribution in the energy equation) is studied. Initiation of combustion is effected by two models of ignition: 1) simulation of spark ignition (what minimum enthalpy-augmentation of a given duration at one wall leads to self-sustained propagation of flame across the charge), and 2) simulation of hot-kernel ignition (what minimum enthalpy-augmentation of a given volume at one specific internal site leads to self-sustained flame propagation).

Nomenclature

$B^{*\prime}$ = preexponential constant for reaction rate
c_p^* = specific heat capacity at constant pressure
c_v^* = specific heat capacity at constant volume
D^* = binary diffusion coefficient
D = D^*/D_u^*
D_u^* = value of D^* in initial, unburned premixture
f = premultiplier, pressure-derivative term of energy equation
$H(t)$ = Heaviside unit step function
K = $(T_b^* - T_u^*)/T_u^*$
$L^*(t^*)$ = spatial separation of parallel walls
L_0 = $L^*(0)/(D_u^*/u_u^*)$
Le = $(\lambda^*/c_p^*)/(\rho^* D^*)$, taken constant
m^* = $m_O^* \nu_O + m_N^* \nu_N + m_F^* \nu_F$
m_i^* = molecular weight of species i
n = exponent for pressure dependence of $\rho^2 D$
$p^*(t^*)$ = pressure
$p(t)$ = $p^*(t)/p_u^*$
Q^* = heat of combustion per mass of mixture
R^* = $c_p^* - c_v^*$
t^* = time since start of enthalpy addition
t = $t^*/(D_u^*/u_u^{*2})$
$T^*(\psi^*,t^*)$ = temperature
$T(\psi,t)$ = $[T^*(\psi^*,t^*) - T_u^*]/(T_b^* - T_u^*)$
$T_p(t)$ = temperature prescribed at wall near ignition [see Eq. (11)]
$T_w(t)$ = temperature prescribed at wall away from ignition [see Eq. (10)]
T_w^0 = see Eq. (12)
T_b^* = $T_u^* + (Q^*/c_p^*) Y_{Fu}$
T_u^* = value of T^* in initial, unburned premixture
$u^*(\psi^*,t^*)$ = gas speed in x^* direction
$u(\psi,t)$ = $u^*(\psi^*,t^*)/u_u^*$
u_u^* = adiabatic flame speed in initial, unburned premixture
$x^*(\psi^*,t^*)$ = Cartesian space coordinate
$x(\psi,t)$ = $x^*(\psi^*,t^*)/(D_u^*/u_u^*)$
$\tilde{Y}_i(\psi^*,t^*)$ = mass fraction for species i
$Y_i(\psi,t)$ = $m^* \tilde{Y}_i(\psi,t)/(m_i^* \nu_i)$
$Y(\psi,t)$ = $Y_F(\psi,t)/Y_{Fu}$
Y_{Fu} = value of Y_F in initial, unburned premixture
α = exponent for pressure dependence of reaction rate
β = $\Theta^*/(T_b^* - T_u^*)$
γ = c_p^*/c_v^*
Θ^* = Arrhenius activation temperature
λ^* = thermal conductivity
Λ = $B^{*\prime}(D_u^*/u_u^{*2})(p_u^*/R^*)^{\alpha} \Phi^{-\nu_O} Y_{Fu}^{\alpha} \exp(-\beta)$
ν_i = stoichiometric coefficient for species i
$\rho^*(\psi^*,t^*)$ = density
$\rho(\psi,t)$ = $\rho^*(\psi^*,t^*)/\rho_u^*$
ρ_u^* = value of ρ^* in initial, unburned premixture
ϕ = Y_{Fu}/Y_{Ou}; here, $\phi < 1$
Φ = $\phi/(1-\phi)$
ψ^* = stream function
ψ = $\psi^*/(\rho_u^* D_u^*/u_u^*)$

Superscript

$(\,)^*$ = dimensional quantity

Subscripts

F = fuel vapor
i = gas species i (i = O, N, F, or P)
N = nitrogen
O = oxygen

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P = product gas
u = (known) value in initial, unburned premixture (except for u_u^*)

I. Introduction

THIS paper is the first of a two-part theoretical study[13,14] to elucidate properties of laminar unsteady flame propagation through a fuel-lean gaseous premixture, confined in an impervious enclosure with noncatalytic walls. In this first part, the special case of an enclosure of constant volume is considered; the second part is to examine the case in which one of the walls moves in a prescribed manner. The case of predominant interest is that of total mass in the enclosure invariant with time. These studies are motivated by combustion in the cylinder of a homogeneous-charge, spark-ignition, four-stroke (Otto-cycle-type) engine, although innovative technology related to low-heat-transfer, ceramic-capped components will be discussed as well.

Some pertinent existing studies omit flame structure and diffusion in favor of a propagating discontinuity of dynamic and thermodynamic variables; the discontinuity is the site of heat addition by exothermic chemical reaction, the unburned gas undergoing isentropic compression, and the burned gas undergoing either isentropic compression or perfect mixing.[1,2] Such studies, which require input as to how the flame speed varies with the thermodynamic state of the unburned gas, can furnish the pressure change in time in the enclosure and, thus, are appropriate for performance comparisons; further, for near-stoichiometric mixtures, in which NO_x generation is the major environmental constraint, such studies have been modified to furnish insight into the dependence of emissions levels with engine-parameter variation. However, for the appreciably fuel-lean operation of interest here, unburned-hydrocarbons emissions are the major environmental constraint, and the roles of convective, diffusive, reactive, and compressive phenomena in hydrocarbon-air combustion should be retained. These phenomena are central to the nature of reaction-rate retardation near cylinder walls, conventionally maintained relatively cool for materials reasons; unburned hydrocarbons persist near cooled walls, due to quench-layer generation in large-activation-energy premixtures,[3] failure of flame to propagate into crevices,[4] and absorption of gaseous fuel into the oil film coating cooled cylinder walls.[5] In brief, it is necessary to retain finite-rate kinetics, and resolve events on the diffusive scale, temporally and spatially, for present purposes. It is also evident that heat transfer through cooled isothermal walls is essential; adiabatic models[6,7] do not serve present purposes.

Three simplifications are adopted. The first entails adoption of a formulation common in engineering-type investigations of combustion, the Shvab-Zeldovich approximation. Binary diffusion, constant Lewis-Semenov number, constant universal heat capacity, comparable molecular weight for all species (taken as ideal gases), simple variation of transport properties with thermodynamic state, direct one-step irreversible chemical mechanism, etc., are adopted. One generalization is that, just as the orders of reaction with respect to fuel and oxygen in the reaction-rate expression for the one-step pseudomechanism are assigned plausible values (rather than the orders compatible with rigorous one-step stoichiometry), so the exponent on the pressure dependence of the rate expression is taken as adjustable. Another is that the pressure is taken as temporally changing, but spatially invariant. This approximation suppresses acoustic-wave-scale effects and minor spatial inhomogeneity of the pressure field, of negligible practical significance for present purposes (cf., Refs. 7-9); only with the onset of knock does spatial inhomogeneity of the pressure field enter significantly.

The second simplification is that a simple spatially one-dimensional Cartesian-type geometry is examined. This geometry is relevant to certain rapid-compression-machine-type laboratory apparatus.

The third simplification is the retention of a laminar formulation, again pertinent only to the rapid-compression machine.

A major goal of the present constant-volume study of combustion of a confined premixture is to elucidate the relative importance of the three effects arising from a temporally variant pressure field; namely, 1) that effect associated with the distinction of entropy and enthalpy in the second law of thermodynamics (henceforth, for brevity, alluded to as the explicit-temporal-derivative effect); 2) that effect in the diffusive terms associated with the variation of transport properties with thermodynamic state; and 3) that effect in the chemical-reaction terms associated with the variation of reaction rate with pressure. Thus, for insight, each of these phenomena is "turned on" individually, as well as in the several possible combinations, in the studies presented here.

Another goal is to elucidate parameters for simulation of the spark event for combustion in an enclosure. Within the Shvab-Zeldovich context, electrical (especially, ionizing) and photochemical (especially, dissociative) properties of the spark kernel are ignored, and the spark is modeled simply as a transient enthalpy addition occurring at or near a wall. More explicitly, the temperature at one wall is abruptly increased to another constant value, then abruptly returned to its original constant value. For each of several given durations of augmentation, what is sought is the value of the temperature required to achieve a flame propagation that is self sustaining. For comparison, the spatial extent and strength of a volume-distributed enthalpy source is briefly examined as well. In most (but not all) instances, sharp delineation of enthalpy-addition requirements for flame propagation proves possible, i.e., a go/no-go criterion is often definable.

Finally, it is noted that the solution to the (transcendentally) nonlinear parabolic boundary/initial-value problem to be formulated is obtained numerically by means of method-of-lines integration with spline interpolation. This standard and efficient procedure has been discussed previously in the literature[10,11] and has been employed previously by the authors.[5] The only restriction worth noting is that, in the form used here, the initial conditions must be taken compatible with the boundary conditions.

II. Formulation

A similar formulation to the one given below was developed by Sirignano,[6] but generalizations in constraints permit examination of surface ignition and wall quench, and discussion of end-gas knock.

For a direct one-step irreversible exothermic chemical reaction between fuel F and oxidant O that generates product P, i.e.,

$$\nu_N N + \nu_O O + \nu_F F \rightarrow \nu_N N + \nu_P P \tag{1}$$

in the Shvab-Zeldovich approximation, under a von Mises transformation, the nondimensional fuel-conservation and energy-conservation equations for nonsteady one-dimensional low-Mach-number reacting flow are

$$\frac{\partial Y}{\partial t} - p^n \frac{\partial^2 Y}{\partial \psi^2} = -\Lambda p^\alpha Y^{\nu_F} (1+\Phi Y)^{\nu_O} \exp\left\{-\beta \frac{(1-T)}{T}\right\} \tag{2}$$

$$\frac{\partial T}{\partial t} - (Le) p^n \frac{\partial^2 T}{\partial \psi^2} = \Lambda p^\alpha Y^{\nu_F} (1+\Phi Y)^{\nu_O} \exp\left\{-\beta \frac{(1-T)}{T}\right\} + f \frac{\gamma - 1}{\gamma} \frac{(1+KT)}{Kp} \frac{dp}{dt} \tag{3}$$

and the (complementary) nondimensional state, mass-conservation, and mapping equations are

$$\rho = \frac{p}{(1+KT)} \tag{4}$$

$$\frac{\partial u}{\partial \psi}=\frac{\partial}{\partial t}\left(\frac{1}{\rho}\right)=\frac{\partial}{\partial t}\left(\frac{(1+KT)}{p}\right) \tag{5}$$

$$\frac{\partial x}{\partial \psi}=\frac{1}{\rho}=\frac{(1+KT)}{p} \tag{6}$$

In a manner consistent with the accuracy of the Shvab-Zeldovich formulation, in the diffusion terms of Eqs. (2) and (3), it is taken that $\rho^2 D = p^n = \text{fnc}(t)$. The cases $n=0$, 1 are examined in this paper.

In the reaction-rate terms of Eqs. (2) and (3), α characterizes the preexponential pressure dependence. While the choice $\alpha=[(\nu_F+\nu_O)-1]$ is consistent with certain considerations (cf. Ref. 12), the values assigned ν_F and ν_O in the rate expression are not, in general, consistent with the stoichiometry of the one-step pseudomechanism of Eq. (1). Similarly, α is taken to be empirically assignable. For the most part, in Sec. III, ν_F, $\nu_O=1$ is adopted, and the cases of $\alpha=0$, ½, 1 are considered.

Strictly speaking, in the temporal pressure-gradient term of Eq. (3), $f=1$. However, in order to determine the relative effect of pressure variation on the contributing terms in Eqs. (2) and (3), the cases $f=0$, 1 are considered.

From steady fuel-lean laminar flame propagation, for $\beta \gg 1$, the only case of practical interest in an automotive context, it is taken that

$$\Lambda=\beta^{\nu_F+1}[2\Gamma(\nu_F+1)Le^{\nu_F+1}]^{-1}[1+O(\beta^{-1})] \tag{7}$$

where higher order terms are known but are not utilized here.

In this formulation, the fixed wall is located at $x=0$; the moving wall is located at $x=L(t)$, with $L(0)\equiv L_0=\text{const}>1$. Under the von Mises transformation, with the fixed wall located at $\psi=0$, the moving wall is located at $\psi=\Psi(t)$, with $\Psi(0)\equiv\Psi_0=\text{const}>0$, i.e.,

$$\psi=\int_0^x \rho\,dx_1=p\int_0^x \frac{dx_1}{(1+KT)} \tag{8a}$$

$$\Psi=\int_0^L \rho\,dx_1=p\int_0^L \frac{dx_1}{(1+KT)} \tag{8b}$$

In general, the initial conditions for this flow geometry are those for a cold, unburned premixture; namely,

$$Y\to 1,\ T\to 0\ (p\to 1)\quad \text{as } t\to 0$$
$$(0<x<L_0 \text{ and/or } 0<\psi<\Psi_0) \tag{9}$$

Note that, subject to Eq. (9), it follows, from Eq. (8), that $\Psi_0=L_0$.§ One possible (but not examined) exception to Eq. (9) is introducing stratification so that $Y\to\text{fnc}(\psi)\neq 1$ as $t\to 0$. An exception to Eq. (9), which is examined below, is the introduction of a hot spot to simulate a volumetric addition of enthalpy as an igniting kernel, such that $T\to T_0(\psi)\neq 0$ as $t\to 0$. In general, the boundary conditions, assuming that both walls are impermeable noncatalytic ones, are

$$\frac{\partial Y}{\partial \psi}\to 0,\quad T\to T_w=\text{fnc}(t)\ \text{ as }\ \psi\to 0\ (t>0) \tag{10}$$

$$\frac{\partial Y}{\partial \psi}\to 0,\quad T\to T_p=\text{fnc}(t)\ \text{ as }\ \psi\to L_0\ (t>0) \tag{11}$$

§While blow-by, with Ψ a prescribed (decreasing) function of t, could be treated, here it is taken that the total mass is constant: $\Psi=\Psi_0=L_0$, const, for all t.

Table 1 Minimum temperature T_w^0 for self-sustaining flame[a]

Case depicted in	$D(n)$	RR(α)	$p(f)$	$(T_w^0)_{\min}$
Fig. 1	1(0)	1(0)	No(0)	2.0
Fig. 2	p(1)	1(0)	No(0)	2.5
Fig. 3	1(0)	1(0)	Yes(1)	1.4
Fig. 4	p(1)	1(0)	Yes(1)	1.4
Fig. 5	1(0)	p(1)	Yes(1)	1.0
Fig. 6	p(1)	p(1)	Yes(1)	1.0
Fig. 9	p(1)	$p^{1/2}$(½)	Yes(1)	1.15

[a]Enhanced enthalpy maintained for one-half of a diffusive time scale (D_u^*/u_u^{*2}), where D_u^* is the mass-transfer coefficient of the cold premixture, and u_u^* its adiabatic flame speed. For all cases, $T_p=T_w=0$.

Here, to effect ignition, the temperature at one wall is given by

$$T_w=T_w^0 H(t-t_1)H(t_2-t) \tag{12}$$

with $0<t_1<t_2$, where $H(z)$ denotes the Heaviside step function. The initiation, t_1, and the duration, (t_2-t_1), of the temperature augmentation are to be specified, as is the augmentation, T_w^0. With respect to the moving-wall temperature distribution, various constant values of T_p are to be considered, with $T_p=0$ the value given primary consideration. Equation (9) is chosen compatible with Eq. (10), subject to Eqs. (12) and (11); for $t_1=0$, Eq. (9) should be modified very near $\psi=0$. For this latter case, the temperature initial conditions in Eq. (9) might be replaced by

$$T\to T_0(\psi)=T_w^0(1-(\psi/\epsilon))H(1-(\psi/\epsilon))$$
$$\text{as } t\to 0\ \ (0<\psi<L_0)$$

with $0<\epsilon\ll 1$.

From integration of the mapping equation (6), it is determined that the pressure is related to the integral of the temperature distribution by

$$p=\frac{L_0}{L}\left(1+\frac{K}{L_0}\int_0^{L_0} T\,d\psi\right)=\frac{L_0}{L}(1+I) \tag{13a}$$

The logarithmic derivative, with respect to t, of this relation is

$$\frac{1}{p}\frac{dp}{dt}=-\frac{1}{L}\frac{dL}{dt}+\frac{1}{(1+I)}\frac{dI}{dt} \tag{13b}$$

In Eq. (13), $L=\text{fnc}(t)$ (to be specified). It is evident that reduction of the boundary/initial-value problem to two equations for two unknowns, $Y(\psi,t)$ and $T(\psi,t)$, leads to an integrodifferential equation. Iteration in numerical solution is avoided by treatment of the (temporal) pressure gradient term as a forcing function, i.e.,

$$\frac{1}{p(t_j)}\frac{dp}{dt}(t_j)=-\frac{1}{L(t_j)}\frac{dL}{dt}(t_j)$$
$$+\frac{[I(t_{j-1})-I(t_{j-2})]/(t_{j-1}-t_{j-2})}{1+(\tfrac{1}{2})[I(t_{j-1})+I(t_{j-2})]} \tag{14a}$$

where

$$I(t_k)=\frac{K}{L_0}\int_0^{L_0} T(\psi,t_k)\,d\psi \tag{14b}$$

and where $t_j>t_{j-1}>t_{j-2}$, $j=2,3,4,\ldots$, but the time intervals are small. The contribution of the second term at $j=0$, 1 is neglected. While a more accurate finite difference approximation is readily derived, the adequate numerical accuracy of the simplistic treatment just enumerated has been indicated.[13]

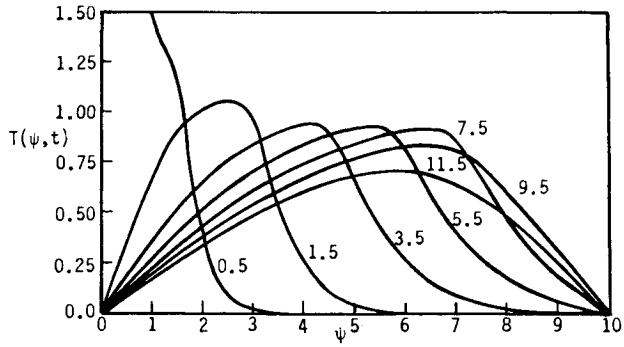

Fig. 1 Temperature T as a function of the stream function ψ for several times ($t=0.5$, 1.5, etc.) since ignition at $t=t_I=0$; for the depicted case of minimal wall enthalpy for self-sustaining flame propagation, $t_2=0.5$, $T_w^0=2.0$, $n=\alpha=f=0$.

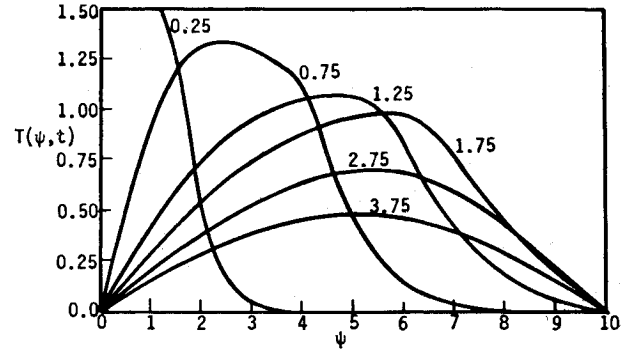

Fig. 2 Same as Fig. 1, except $T_w^0=2.5$, $n=1$.

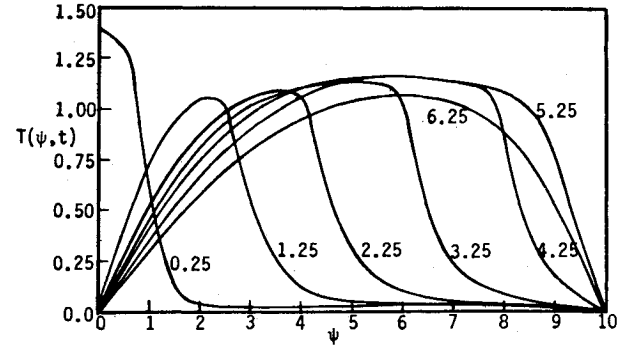

Fig. 3 Same as Fig. 1, except $f=1$, $T_w^0=1.4$. For $t>4.25$, flame propagation transforms to residual-fuel burn-up, as the peak temperature no longer approaches the wall.

III. Results

The effects of pressure variation on the diffusion coefficient (here, $n=0,1$, alternatively designated $D=1,p$), or pressure on the reaction rate (here, $\alpha=0,\frac{1}{2},1$, alternatively designated RR$\sim 1,p^{\frac{1}{2}},p$) and of the explicit temporal derivation of pressure (here, $f=0,1$, alternatively designated $\dot{p}=$ no, yes) can be examined for three different standard ignition problems, which are 1) the minimum, temporally constant temperature level that must be maintained for a specified time interval at one wall to generate a self-sustaining flame propagation through the confined premixture, 2) the minimum time interval required for a specified constant temperature to be applied at one wall to generate a self-sustaining flame propagation through the confined premixture, and 3) the minimum (almost) spatially constant temperature level that must be applied over a specified spatial interval within the confining volume for a self-sustaining flame propagation through the confined premixture. While all three cases have been con-

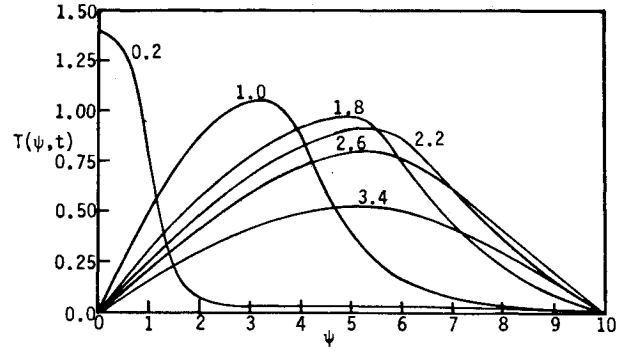

Fig. 4 Same as Fig. 1, except $n=f=1$, $T_w^0=1.4$.

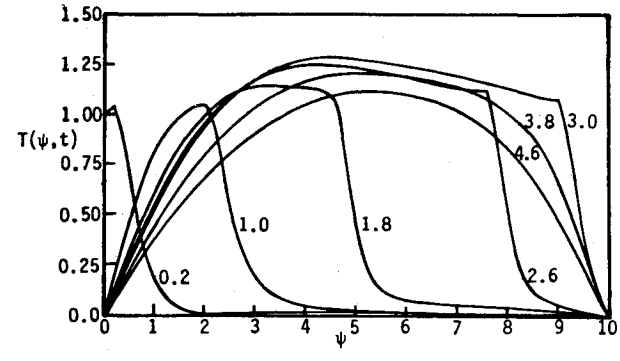

Fig. 5 Same as Fig. 1, except $\alpha=f=1$, $T_w^0=1.0$.

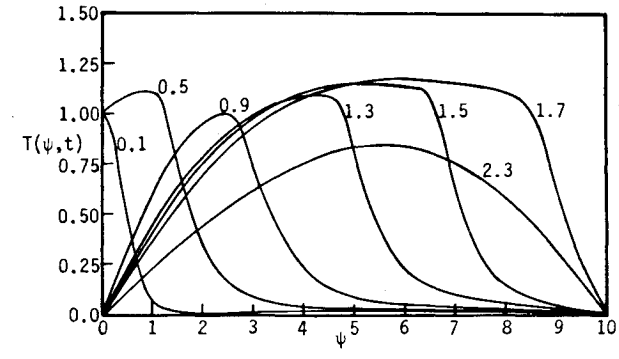

Fig. 6 Same as Fig. 1, except $n=\alpha=f=1$, $T_w^0=1.0$.

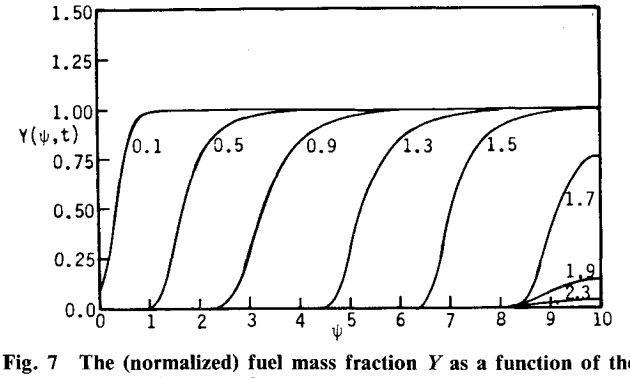

Fig. 7 The (normalized) fuel mass fraction Y as a function of the stream function ψ presented at several times since ignition for the case of Fig. 6. At 2000 rpm, roughly 15 ms separate combustion and blowdown in an Otto-cycle cylinder. Since the adopted nondimensional (diffusive) time scale is roughly 0.1 ms, the available 150 time units are fully adequate for residual-fuel burn-up. Hence one-wall quenching is not the source of exhausted hydrocarbons,[16] if a laminar model suffices, even with expansional cooling and heat transfer during the power stroke.

sidered by the investigators, because of the multitude of parametric variations (and possible boundary conditions at the wall far from the ignition site), only the first and third modes are represented in the figures and tables included here. Incidentally, a typical case to be reported required about 1 min on a CDC Cyber 175 computer; thus, the rich variety of aerothermochemical phenomena included within the boundary/initial-value problem, far from exhaustively pursued here, may be explored further quite feasibly.

The following parametric values are terms nominal for brevity of reference, and are held invariant throughout the calculations to be reported (except where explicitly noted): $\nu_O = \nu_F = 1$, $\beta = 10$, $Le = 1$, $\gamma = 1.4$, $t_1 = 0$, $L_0 = 10$, $T_w = 0$, $\Phi = 1$, and $K = 7$.

It should be appreciated at the outset that simplistic division into go/no-go alternatives is convenient for categorizing whether a given set of parametric values gives rise to a self-sustaining flame propagation through the premixture or not; however, in practice, there are borderline cases in which a weak, relatively low-temperature flame consumes the preponderance of fuel for the specified domain in a relatively short time (say, on the order of 10 diffusive time scales), but well might not do so for even moderately larger values of L_0.

It may be anticipated, for the present constant-volume, chemically exothermic cases in which pressure in general rises in time, that assigning $n = 1$ (as opposed to $n = 0$) gives rise to a spatially thicker flame than arises for the more commonly considered laminar isobaric flame; heat diffuses more readily across the charge, and out of the flow domain if the boundaries are cold relative to the gaseous contents. Clearly, the reaction rate increases with pressure for $\alpha > 0$ and the presence of the explicit pressure derivative ($f = 1$) contributes to the temperature rise, so it is quantitative characterization of these terms that is of interest.

In the first group of cases, the minimum temperature at the ignition wall $(T_w^0)_{\min}$ is sought for a self-sustained flame propagation, for a duration of enhanced wall enthalpy of one-half a diffusive time scale. That is, in Eq. (12), which holds at $\psi = 0$, it is adopted that $t_2 = 0.5$, $t_1 = 0$, so that $T_w = 0$ for $t > 0.5$. A sequence of values is assigned T_w^0 until the minimum value $(T_w^0)_{\min}$ is identified. The boundary conditions (11) holding at the far wall, i.e., at $\psi = L_0$, are taken in the form $T_p = 0$. For the nominal set of parametric values, with $\Lambda = 50$ according to Eq. (7), results are summarized in Table 1. These results are illuminated by Figs. 1-14.

The high value, $(T_w^0)_{\min} = 2.0$, arises for the isobaric-like treatment of the nonisobaric problem, with $n = \alpha = f = 0$ (Fig. 1); restoring (Fig. 2) the effect of pressure on the diffusion coefficient only ($n = 1$, $\alpha = f = 0$) raises $(T_w^0)_{\min}$ to 2.5, and the time required for the flame to traverse the domain is reduced to very roughly one-third of the value in Fig. 1. Moreover, in Fig. 2 the burn-up is characterized by a maximum temperature (over ψ) that monotonically decreases with increasing time, whereas in Fig. 1 the maximum temperature reaches a plateau until the fuel is exhausted. If one takes $n = \alpha = 0$, $f = 1$, then $(T_w^0)_{\min} = 1.4$ (Fig. 3); restoring $n = 1$, for $\alpha = 0$, $f = 1$ again gives $(T_w^0)_{\min} = 1.4$ (Fig. 4). However, comparison of Fig. 3, which seems reminiscent in many respects of *isobaric* quenching of a premixed flame approaching a cold impervious noncatalytic wall, with Fig. 4 reveals again that enhanced diffusive transfer greatly reduces the temporal interval for preheating of the premixture in the vicinity of the far wall. The same trend is repeated upon comparison of the case $n = 0$, $\alpha = f = 1$ (Fig. 5), with the case $n = \alpha = f = 1$ (Fig. 6): while $(T_w^0)_{\min} = 1.0$ for both cases, the flame propagation time is reduced when the diffusive transfer is enhanced. Presence of an appreciable explicit dependence of the reaction rate on pressure results in a significantly more sharply defined flame, because the more rapidly propagating flame affords less time for preheating. The presence of a rather well-defined flame is evidenced further by Fig. 7, in which profiles of the (stoichiometrically adjusted and normalized) fuel mass fraction for the case presented in Fig. 6, i.e., $n = \alpha = f = 1$, are given.

To this point thermal and fuel mass fraction profiles have been given for the critical case, i.e., for that minimum value of T_w^0 for which self-sustained flame propagation follows a half-diffusive-time-scale wall heating. As already noted, there are

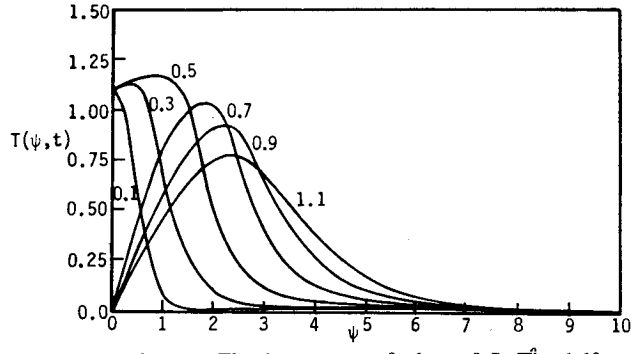

Fig. 8 Same as Fig. 1, except $n = f = 1$, $\alpha = 0.5$, $T_w^0 = 1.10$.

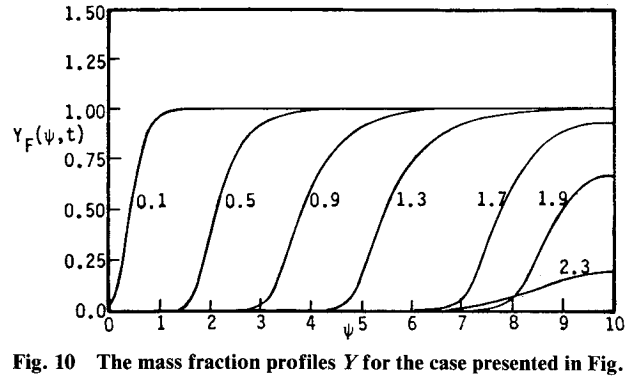

Fig. 10 The mass fraction profiles Y for the case presented in Fig. 9.

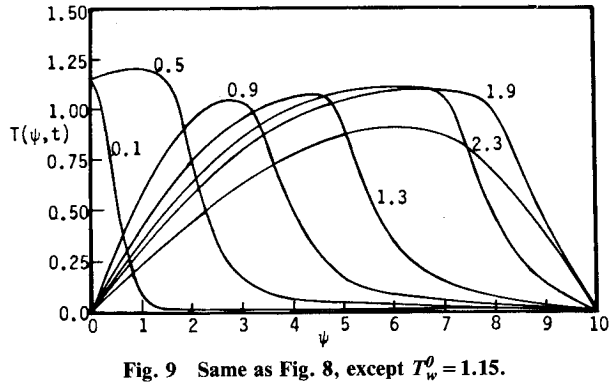

Fig. 9 Same as Fig. 8, except $T_w^0 = 1.15$.

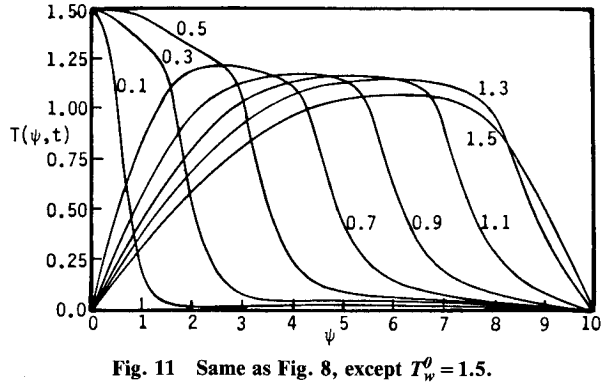

Fig. 11 Same as Fig. 8, except $T_w^0 = 1.5$.

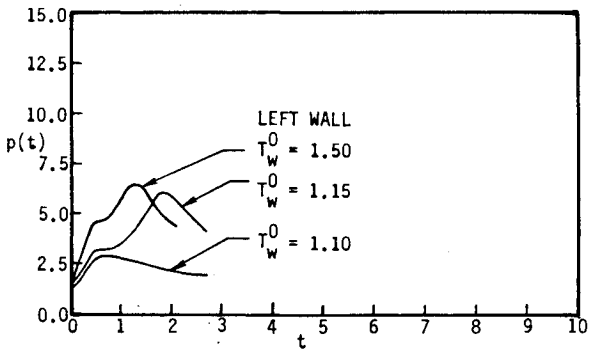

Fig. 12 The pressure p, normalized against its initial value, presented as a function of time t for the three cases presented in Figs. 8, 9, and 11 for which $T_w^0 = 1.10$, 1.15, and 1.50, respectively. For all three cases, $n = f = 1$, $\alpha = 0.5$.

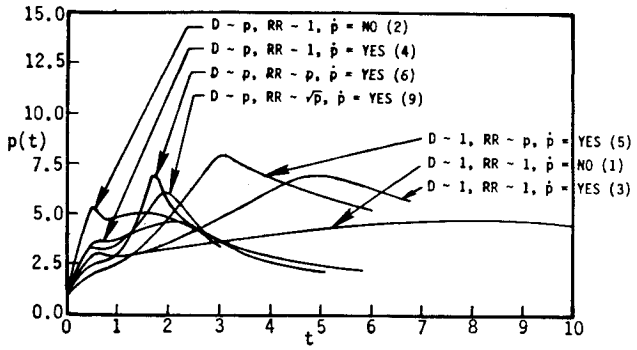

Fig. 14 The pressure p as function of time t, for most of the previous figures. (The numbers in parentheses identify the figure in which the associated thermal profiles were plotted as a function of stream function at several selected times.)

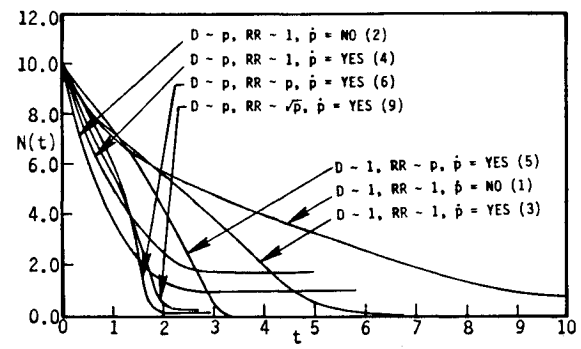

Fig. 13 The net remaining fuel N (actually, the integral of Y over ψ) presented as a function of time t, for most of the previous figures. (The numbers in parentheses identify the figure in which the associated thermal profiles were plotted as a function of stream function at several selected times.)

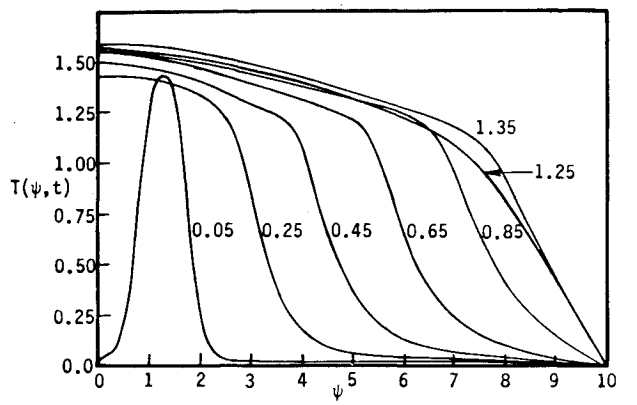

Fig. 15 For the nominal case, except that $\phi = 0.8$ so $\Lambda = \phi/(1-\phi) = 4$ and $\Lambda = 41.6$, with $n = 1$, $\alpha = 0$, $f = 1$, the temperature T given as a function of stream function ψ for several times. The early-time profile at $t = 0.05$ suggests the nature of the volumetric "hot spot" near the adiabatic wall at $\psi = 0$ used to effect ignition. The far wall at $\psi = 10$ is held at $T = 0$ for all time. The compressive heating of the burned gas results in monotonically rising temperature with distance behind the flame.

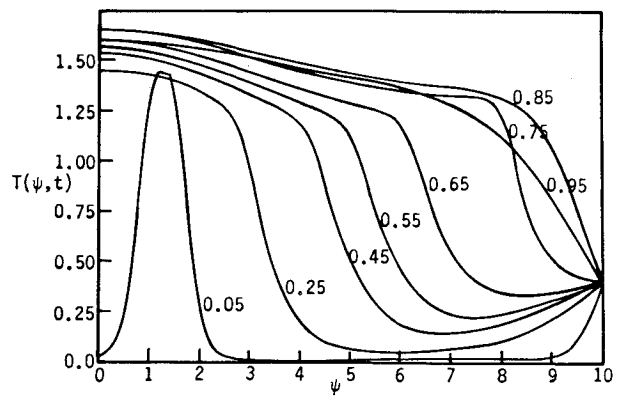

Fig. 16 Same as Fig. 15, except $T(10,t) = 0.4$. The preheating by a wall held at four-tenths of the increment of the adiabatic flame temperature over the cold-premixture temperature has modest effect.

cases (e.g., those of Figs. 1 and 2) for which definition of the go/no-go criterion is not well defined. An example of a well-defined criterion is afforded by Figs. 8-11, for all of which $n = 1$, $\alpha = 0.5$, $f = 1$. Whereas $T_w^0 = 1.10$ gives no self-sustaining flame (Fig. 8), $T_w^0 = 1.15$ does (Figs. 9 and 10). Setting $T_w^0 = 1.5$ gives more vigorous burning (Fig. 11). By the criterion used here, $(T_w^0)_{\min} = 1.15$ for this case. Comparison of Figs. 6 and 9 reveals that varying α from 0.5 to 1.0 alters the "minimal-condition" flame only slightly. Figure 12 presents the pressure (nondimensionalized against its initial value) as a function of time for $T_w^0 = 1.10$, 1.15, and 1.5; while the enclosed volume depressurizes in time due to heat transfer, clearly the relative failure to achieve much enhancement in pressure for $T_w^0 = 1.10$ is evident.

In Fig. 13, the total integrated fuel remaining $N(t)$ is presented as a function of time t for cases for which temperature and fuel-mass-fraction profiles have been presented. It is seen that in three cases complete oxidation of the fuel does not occur, although at least 80% of the initial fuel is consumed in all cases. Clearly, taking $n = 1$ (rather than $n = 0$) is particularly significant. In Fig. 14, it is seen that the pressure peak is achieved earlier for $n = 1$ (than for $n = 0$), but the value of the peak is related less easily to other parameter assignments.

In the second set of cases, parameters are assigned nominal values except that $\phi = 0.8$, so $\Phi = \phi/(1-\phi) = 4$; also Λ is assigned the slightly revised value of 41.6. An adiabatic condition holds uniformly in time at $\psi = 0$, and an isothermal or adiabatic condition holds uniformly in time at $\psi = L_0$. In all cases, $n = 1$, $\alpha = 0$, $f = 1$. Ignition is achieved identically in all cases: the temperature is appreciably enhanced (to the same value over the same expanse) in a region near $\psi = 0$. In Figs. 15-19, profiles are presented for cases in which the far wall at $\psi = L_0$ is held at temperatures of 0.0, 0.4, 0.6, and 0.8; while far-wall heating of the nearby premixtures tends to hasten fuel burn-up, holding the far wall at 0.8 rapidly results in a surface-initiated flame propagation such that the peak of the fuel-mass-fraction profile does not occur at the far wall. According to Fig. 20, the result of having the far wall of adiabatic character is a compressive preheating and rapid conversion of the residual charge. The associated profiles for $N(t)$

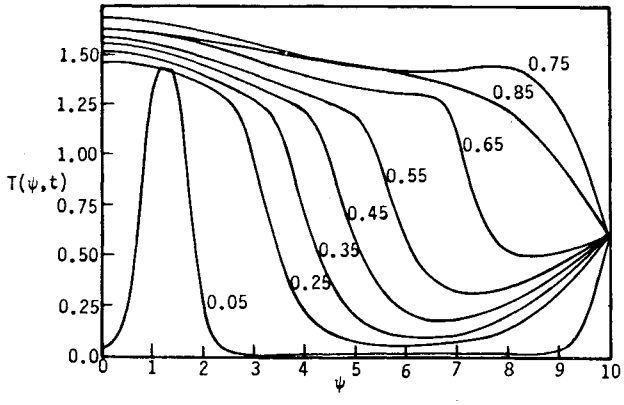

Fig. 17 Same as Fig. 15, except $T(10,t) = 0.6$.

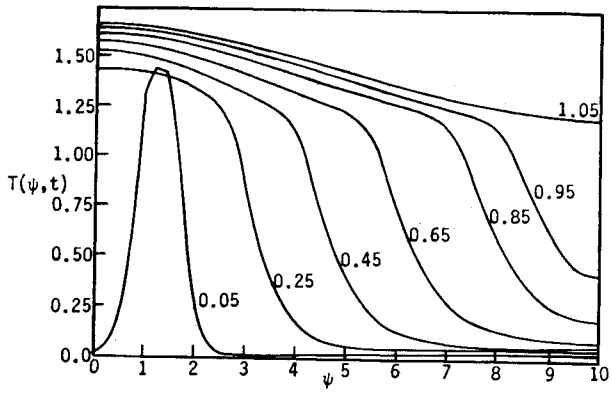

Fig. 20 Same as Fig. 15, except $\partial T(10,t)/\partial\psi = 0$.

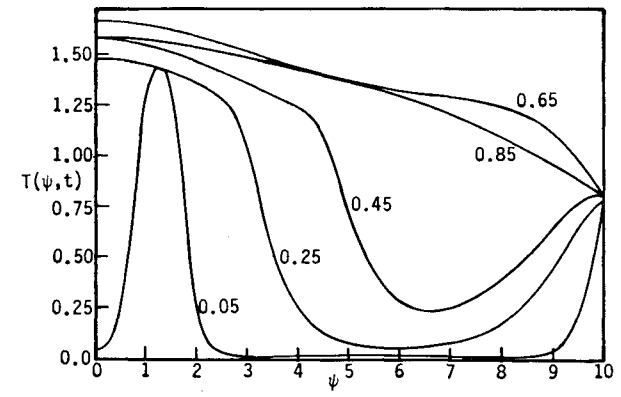

Fig. 18 Same as Fig. 15, except $T(10,t) = 0.8$. A surface ignition is effected before the original flame crosses the charge.

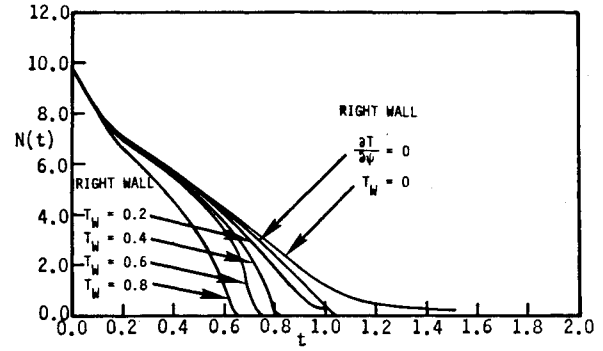

Fig. 21 The net remaining fuel N presented as a function of time t for the cases described in Figs. 15-20. Enthalpy addition tends to result in faster burning than adiabaticity.

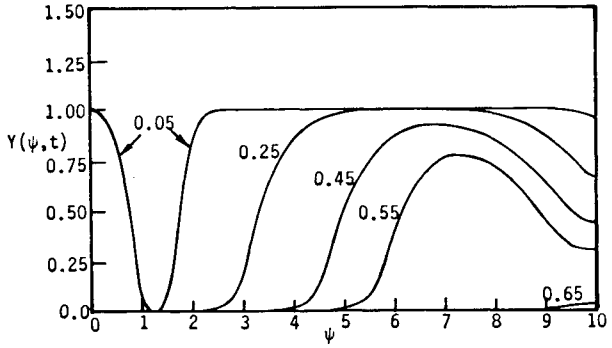

Fig. 19 The (normalized) fuel mass fraction Y presented as a function of the stream function ψ at several times, for the case of Fig. 17. At some times, the peak fuel value occurs away from the far wall at $\psi = 10$, as evidence of surface-initiated burning.

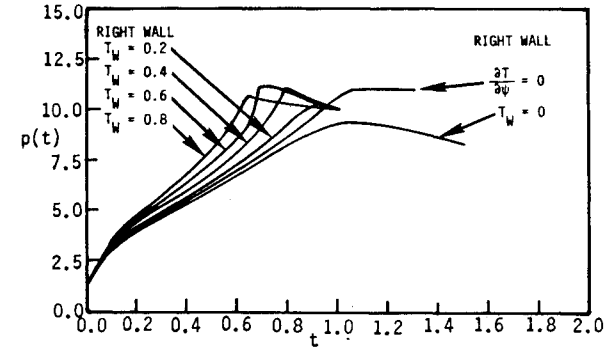

Fig. 22 The dimensionless pressure p presented as a function of time t for the cases described in Figs. 15-20. The absence of depressurization in the adiabatic case is noteworthy.

and $p(t)$ are given in Figs. 21 and 22, respectively.

The third set of cases is carried out for the same conditions as the second set, except that the value of α is increased from zero to unity.[13] The reaction front is appreciably "steepened" and the time for conversion to product is reduced. For adiabatic walls, isentropic compression heats the unburned and burned gas, and the roles of reaction and diffusion are mostly confined to the (propagating) flame, which occupies a subdomain of the enclosed volume.

IV. Concluding Remarks

One phenomenon not well delineated in the results presented here is the almost spatially homogeneous conversion of residual charge to product, an explosion (rather than flame propagation) referred to in an automotive context as end-gas knock.[14] This phenomenon occurs for conditions in which compressive preheating of the residual charge is excessive, and results in the breakdown of the approximation of a spatially homogeneous pressure field (because chemical-conversion time is less than acoustic-equilibration time). A major reason why this phenomenon is not observed here is due to the limited expanse of the above-studied domain, i.e., due to the values of L_0 to which attention has been confined. Efficient numerical treatment of appreciably larger values of L_0 entails effective use of adaptive gridding, so that refined spatial resolution is introduced only where it is needed; the alternative procedure is to adopt limit-process expansions of singular perturbation to capitalize upon the largeness of the dimensionless Arrhenius activation temperature.[14] Thus, while insight into nonisobaric effects on propagation of a one-dimensional laminar flame

between parallel walls (including the role of enhanced diffusive transfer) has been afforded, some practically important phenomena may remain inaccessible. However, it seems worth emphasizing that even the parametric variations examined would not have been feasible without adopting a familiar and highly plausible extension of the conventional Shvab-Zeldovich approximation for nonisobaric combustion, specifically, the taking of the pressure to be a function of time only (in the absence of applied spatial gradients). Within this approximation, further investigation of combustion within a variable-volume enclosure (from prescribed motion of, say, the wall furthest from the ignition site) may be pursued with modest computational requirements.[14,15]

Acknowledgments

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References

[1]Lavoie, G. A., Heywood, J. B., and Keck, J. C., "Experimental and Theoretical Study of Nitric Oxide Formation in Internal Combustion Engines," *Combustion Science and Technology*, Vol. 1, 1970, pp. 313-326.

[2]Carrier, G. F., Fendell, F. E., and Feldman, P. S., "Nonisobaric Flame Propagation," *Dynamics and Modeling of Reactive Systems*, Academic Press, New York, 1980, pp. 333-352.

[3]Carrier, G. F., Fendell, F. E., Bush, W. B., and Feldman, P. S., "Nonisenthalpic Interaction of a Planar Premixed Laminar Flame with a Parallel End Wall," SAE Paper 790245, 1979.

[4]Carrier, G. F., Fendell, F. E., and Feldman, P. S., "Interaction of a Planar Laminar Premixed Flame with a Perpendicular Wall," SAE Paper 800285, 1980.

[5]Bush, W. B., Fendell, F. E., and Fink, S. F., "Effect of Boundary Thermal Constraint on Planar Premixed-Flame/Wall Interaction," *Combustion Science and Technology*, Vol. 24, 1980, pp. 53-70.

[6]Sirignano, W. A., "One-Dimensional Analysis of Combustion in a Spark-Ignition Engine," *Combustion Science and Technology*, Vol. 7, 1973, pp. 99-108.

[7]Sorenson, S. C., "Modeling Turbulent Transient Combustion," SAE Paper 780639, 1978.

[8]Westbrook, C.K., "Propagation of the Flame through a Stratified Charge Combustion Chamber," *Acta Astronautica*, Vol. 5, 1978, pp. 1185-1198.

[9]Westbrook, C. K., "Fuel Motion and Pollutant Formation in Stratified Charge Combustion," SAE Paper 790248, 1979.

[10]Sincovec, R. F. and Madsen, N. K., "Software for Nonlinear Partial Differential Equations," *ACM Transactions on Mathematical Software*, Vol. 1, 1975, pp. 232-260.

[11]Sincovec, R. F., "Generalized Collocation Methods for Time-Dependent, Nonlinear Boundary-Value Problems," *Society of Petroleum Engineers Journal*, Vol. 17, 1977, pp. 345-352.

[12]Glassman, I., *Combustion*, Academic Press, New York, 1977.

[13]Fink, S. F., Fendell, F. E., and Bush, W. B., "Nonadiabatic Nonisobaric Propagation of a Planar Premixed Flame: Constant-Volume Enclosure," AIAA Paper 83-0239, Jan. 1983.

[14]Bush, W. B., Fendell, F. E., and Fink, S. F., "Modeling End-Gas Knock in a Rapid-Compression Machine," AIAA Paper 84-0208, Jan. 1984.

[15]Carrier, G., Fendell, F., Fink, S., and Feldman, P., "Heat Transfer as a Determent of End-Gas Knock," *Combustion Science and Technology*, Vol. 38, 1984, pp. 1-48.

[16]Dyer, T. M., "Sources of Unburned Hydrocarbon Emissions from Homogeneous-Charge Automotive Engines," Sandia National Laboratories, Livermore, Calif., SAND83-8241, Sept. 1983.