Modeling End-Gas Knock in a Rapid-Compression Machine

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A rapid-compression machine is a laboratory apparatus to study aspects of the compression stroke, combustion event, and expansion stroke of an Otto cycle engine. As a simple model of such a machine, unsteady one-dimensional nonisobaric laminar flame propagation through a combustible premixture, enclosed in a variable volume, is examined in the asymptotic limit of an Arrhenius activation temperature large relative to the conventional adiabatic flame temperature. In this limit, a thin propagating flame separates the nondiffusive expanses of the burned and unburned gases. The pressure through the enclosure is spatially homogeneous for smooth flame propagation. However, expansion of the hot burned gas results in compressional preheating of the remaining unburned gas and, in fact, the spatially homogeneous gas may undergo autoconversion prior to the arrival of the propagating flame. If such an explosion is too rapid for acoustic adjustment, large spatial differences in pressure arise and the resulting nonlinear waves produce audible knock. Here, attention is concentrated on what fraction (if any) of the total charge may undergo autoconversion for a given operating condition and what enhanced heat transfer from the end gas would preclude autoconversion—although too great a heat transfer from the end gas could result in flame quenching (unburned residual fuel).

I. Introduction

DURING nonisobaric flame propagation through an initially homogeneous premixture of combustible gases in an (in general, variable-volume) enclosure, end-gas knock may occur. That is, the residual unburned gas is preheated by compression prior to the arrival of the flame, owing to expansion of the already burned gas and possibly also owing to the movement of the walls of the enclosure. If this preheating results in a high enough unburned-gas temperature, virtually the entire residual gas may undergo autoignition and rapid conversion to product in a spatially homogeneous explosion. This phenomenon is known as end-gas knock; because the temporal scale of the abrupt local autoconversion may be shorter than the acoustic wave speed, the pressure field (well approximated to be a function of time only during normal flame propagation) becomes spatially nonuniform and the resulting nonlinear waves interact with the walls to produce loud noise. In view of the current capacity to treat the exhaust of Otto cycle engines, the potential damage to engine components from end-gas knock is a major obstacle to operation at high thermal efficiency, i.e., at high compression ratios.[1,2]

In this paper, further insight into end-gas knock is sought from a mechanical engineering point of view, as distinct from a chemical kinetic one. That is, a Shvab-Zeldovich type of formulation§ of the one-dimensional unsteady laminar interplay of species and heat diffusion, exothermic chemical reaction, compressional heating, and heat loss is solved for an impervious noncatalytic variable-volume enclosure. Such a model may suffice for a so-called rapid-compression machine for cases in which ignition is arranged such that a planar flame propagates parallel to one movable (piston-like) end wall. Often, such a machine serves as a conveniently instrumented laboratory apparatus for detailed examination of compression and reaction (and perhaps subsequent expansion as well). In contrast, in an Otto cycle engine, multiple repetitions of the entire cycle (including induction and exhaust) are involved, the flame propagation is highly unsteady ("turbulent"), the flame is often predominantly perpendicular to the piston crown, and the range of parametric variation may in practice be constrained to a relatively narrow range by cost and available equipment.[3,4]

Accordingly, the following questions are addressed: 1) under what conditions is the onset of knock to be expected in a rapid-compression machine? 2) what fraction of the initial premixture undergoes autoconversion? and 3) what heat transfer from the end gas would suffice for smooth flame propagation across the entire combustible mixture?

II. Formulation

For a low Mach number flow in which fuel F and oxygen O pass exothermically to product P (in the presence of nitrogen N) via

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

where ν_i is the stoichiometric coefficient of species i and the dimensional conservation equations for mass, species, and the energy and state equation are taken, in the domain $0<x^*<L^*(t^*)$, $t^*>0$, to be[5,6]

$$\frac{\partial \rho^*}{\partial t^*}+\frac{\partial(\rho^* u^*)}{\partial x^*}=0: \quad \frac{\partial \psi^*}{\partial x^*}=\rho^*, \quad \frac{\partial \psi^*}{\partial t^*}=-\rho^* u^* \tag{2}$$

$$\rho^*\left(\frac{\partial Y_i}{\partial t^*}+u^*\frac{\partial Y_i}{\partial x^*}\right)-\frac{\partial}{\partial x^*}\left[(\rho^* D^*)\frac{\partial Y_i}{\partial x^*}\right]=-w^*,$$

$$i=\mathrm{F},\ \mathrm{O};\ Y_i=m^*\tilde{Y}_i/m_i^*\nu_i \tag{3}$$

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§In particular, a direct one-step irreversible bimolecular second-order Arrhenius-type global reaction is adopted. No attempt is made to examine detailed chemical kinetic rates and mechanisms.

$$\rho^*\left(\frac{\partial T^*}{\partial t^*}+u^*\frac{\partial T^*}{\partial x^*}\right)-\frac{\partial}{\partial x^*}\left(\frac{\lambda^*}{c_p^*}\frac{\partial T^*}{\partial x^*}\right)$$

$$=\left(\frac{Q^*}{c_p^*}\right)w^*+\frac{1}{c_p^*}\frac{\mathrm{d}p^*}{\mathrm{d}t^*} \tag{4}$$

$$p^*=\rho^*R^*T^* \tag{5}$$

where t^* and x^* are the time and Cartesian spatial coordinates, respectively; u^* the gas speed; ψ^* the stream function; ρ^* the density; T^* the temperature, R^* the gas constant for the mixture (taken to be composed of species of comparable molecular weight); p^* the pressure (taken to be a function of time only from consideration of the equation of conservation of momentum); $\tilde{Y}$ and m_i^* the mass fraction and molecular weight, respectively, of species i; $m^*=\nu_F m_F^*+\nu_O m_O^*+\nu_N m_N^*$; D^* and λ^* the mass transfer and thermal conductivity coefficients, respectively; c_p^* the (constant universal) heat capacity at constant pressure; Q^* the heat of combustion per mass of premixture; and w^* the reaction rate. The Lewis-Semenov number is taken as a constant of order unity, i.e.,

$$Le=\frac{(\lambda^*/c_p^*)}{(\rho^*D^*)}=\text{const}\sim\mathcal{O}(1) \tag{6}$$

It is also taken that

$$\rho^{*2}D^*\sim p^{*n}=fnc(t^*) \tag{7}$$

Further, consistent with the nature of the formulation,

$$w^*=B'^*T^{*\alpha}\rho^{*\nu_F+\nu_O}Y_F^{\nu_F}Y_O^{\nu_O}\exp[-T_a^*/(T^*-T_{u0}^*)] \tag{8}$$

where B'^* is the (constant) frequency factor, T_a^* the (constant) Arrhenius activation temperature, T_{u0}^* the uniform initial premixture temperature introduced to modify the Arrhenius factor so as to preclude the "cold-boundary difficulty," and α the pre-exponential thermal dependence of the reaction rate. Here, $\alpha=[(\nu_F+\nu_O)-1]$ is adopted.

It is convenient to adopt the von Mises transformation $(x^*,t^*)\rightarrow(\psi^*,t^*)$, where the stream function ψ^* is defined in Eq. (2). Under this transformation, the species and energy conservation equations (3) and (4) become

$$\frac{\partial Y_i}{\partial t^*}-(\rho^{*2}D^*)\frac{\partial^2 Y_i}{\partial\psi^{*2}}=-B'^*\left(\frac{p^*}{R^*}\right)^{\alpha}Y_F^{\nu_F}Y_O^{\nu_O}$$

$$\times\exp\left[\frac{-T_a^*}{(T^*-T_{u0}^*)}\right],\quad i=\mathrm{F},\ \mathrm{O} \tag{9}$$

$$\frac{\partial T^*}{\partial t^*}-Le(\rho^{*2}D^*)\frac{\partial^2 T^*}{\partial\psi^{*2}}=\left(\frac{Q^*}{c_p^*}\right)B'^*\left(\frac{p^*}{R^*}\right)^{\alpha}Y_F^{\nu_F}Y_O^{\nu_O}$$

$$\times\exp\left[\frac{-T_a^*}{(T^*-T_{u0}^*)}\right]+\frac{T^*}{(c_p^*/R^*)}\frac{1}{p^*}\frac{\mathrm{d}p^*}{\mathrm{d}t^*} \tag{10}$$

The mass conservation and mapping equations are

$$\frac{\partial u^*}{\partial\psi^*}=\frac{\partial}{\partial t^*}\left(\frac{1}{\rho^*}\right),\quad \frac{\partial x^*}{\partial\psi^*}=\frac{1}{\rho^*} \tag{11}$$

For nondimensionalization,

$$t=\frac{t^*}{(L_0^*/u_{u0}^*)},\quad \psi=\frac{\psi^*}{\rho_{u0}^*L_0^*} \tag{12}$$

$$Y(\psi,t)=\frac{Y_F(\psi^*,t^*)}{Y_{Fu}}=\frac{(1-\phi)}{\phi}\left(\frac{Y_O(\psi^*,t^*)}{Y_{Ob}}-1\right)$$

$$T(\psi,t)=\frac{T^*(\psi^*,t^*)-T_{u0}^*}{T_{b0}^*-T_{u0}^*} \tag{13}$$

$$p(t)=\frac{p^*(t^*)}{p_0^*} \tag{14}$$

$$\rho(\psi,t)=\frac{\rho^*(\psi^*,t^*)}{\rho_{u0}^*},\quad u(\psi,t)=\frac{u^*(\psi^*,t^*)}{u_{u0}^*}$$

$$x(\psi,t)=\frac{x^*(\psi^*,t^*)}{L_0^*} \tag{15}$$

where subscript u denotes the unburned premixture conditions, subscript b the burned-state conditions at the flame, and subscript 0 the initial conditions. Specifically, u_{u0}^* is the initial adiabatic flame speed and T_{b0}^* the initial adiabatic flame temperature. Also, $\phi=(Y_{Fu}/Y_{Ou})$ is the equivalence ratio, with $\phi<1$ for the cases of interest; thus, $Y_{Fb}=0$. Hence, with $\Phi=[\phi/(1-\phi)]$ of order unity, $Y_{Ob}=(Y_{Ou}-Y_{Fu})=Y_{Fu}/\Phi$, and $T_b^*=[T_u^*+(Q^*/c_p^*)Y_{Fu}]$ (including $T_{b0}^*=T_{u0}^*+(Q^*/c_p^*)Y_{Fu}$). Note also that $p_0^*=\rho_{u0}^*R^*T_{u0}^*$.

Thus, the nondimensional species and energy equations are, for α, $n=1$ and ν_F, $\nu_O=1$,

$$\frac{\partial Y}{\partial t}-\epsilon p\frac{\partial^2 Y}{\partial\psi^2}=-\frac{1}{\epsilon}\Lambda_0 pY(1+\Phi Y)\exp\left[\frac{-\beta(1-T)}{T}\right] \tag{16}$$

$$\frac{\partial T}{\partial t}-\epsilon Lep\frac{\partial^2 T}{\partial\psi^2}=\frac{1}{\epsilon}\Lambda_0 pY(1+\Phi Y)$$

$$\times\exp\left[\frac{-\beta(1-T)}{T}\right]+\frac{(\gamma-1)}{\gamma}\frac{(1+KT)}{Kp}\frac{\mathrm{d}p}{\mathrm{d}t} \tag{17}$$

where

$$\epsilon=(D_{u0}^*/u_{u0}^*)/L_0^*\ll 1 \tag{18}$$

$$\beta=T_a^*/(T_{b0}^*-T_{u0}^*)\gg 1$$

$$K=(T_{b0}^*-T_{u0}^*)/T_{u0}^*=\mathcal{O}(1)$$

$$\Lambda_0=(B'^*D_{u0}^*/u_{u0}^{*2})(p_0^*/R^*)(Y_{Fu}/\Phi)\exp(-\beta)\gg 1 \tag{19}$$

$$\gamma=c_p^*/c_v^*=c_p^*/(c_p^*-R^*)>1 \tag{20}$$

The nondimensional state, continuity, and mapping equations are

$$\rho=\frac{p}{1+KT},\quad \frac{\partial u}{\partial\psi}=\frac{\partial}{\partial t}\left(\frac{1}{\rho}\right)=\frac{\partial}{\partial t}\left(\frac{(1+KT)}{p}\right) \tag{21a,b}$$

$$\frac{\partial x}{\partial\psi}=\frac{1}{\rho}=\frac{(1+KT)}{p} \tag{21c}$$

From steady (isobaric) fuel-lean laminar flame propagation, for $\beta\gg 1$, it is known that, for $\nu_F=1$,

$$\Lambda_0=\frac{\beta^2}{2Le^2}[1+\mathcal{O}(\beta^{-1})] \tag{22}$$

where the 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 $L(0)\equiv 1$. 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.,

$$\psi=\int_0^x \rho\,dx_1=p\int_0^x \frac{dx_1}{(1+KT)} \tag{23a}$$

$$\Psi=\int_0^L \rho\,dx_1=p\int_0^L \frac{dx_1}{(1+KT)} \tag{23b}$$

In general, the initial conditions for this flow geometry are

$$Y\to 1,\quad T\to 0(p\to 1)\ \text{as}\ t\to 0\ \text{for}\ \psi>\psi_{f0}\to 0 \tag{24a}$$

$$Y\to 0,\quad T\to 1(p\to 1)\ \text{as}\ t\to 0\ \text{as}\ \psi\to(\psi_{f0})- \tag{24b}$$

Note that, subject to Eqs. (24), it follows from Eqs. (23) that $\Psi_0=1$. In general, if both walls are impermeable, noncatalytic, and adiabatic, the boundary conditions are

$$\frac{\partial Y}{\partial\psi},\ \frac{\partial T}{\partial\psi}\to 0,\ x,u\to 0\ \text{as}\ \psi\to 0(t>0) \tag{25a}$$

$$\frac{\partial Y}{\partial\psi},\ \frac{\partial T}{\partial\psi}\to 0,\ x\to L(t),\ u\to L'(t)\ \text{as}\ \psi\to 1(t>0) \tag{25b}$$¶

The jump conditions at the flames are

$$[\![Y]\!]=(Y_b-Y_u)=-1,\quad [\![T]\!]=(T_b-T_u)=1$$
$$\text{at}\ \psi=\psi_f(t) \tag{26}$$

III. External Hydrodynamics of Flame Propagation

Exterior to the thin-flame structure, there is an unburned region, defined by $\psi_f(t)<\psi<1$, and a burned region, defined by $\psi_f(t)>\psi>0$. In both of these unburned and burned regions, the diffusion and reaction rate contributions are taken to be negligible, so that the species and energy equations (16) and (17) reduce to

$$\frac{\partial Y}{\partial t}=0 \tag{27}$$

$$\frac{\partial T}{\partial t}-\frac{(\gamma-1)}{\gamma}\frac{(1+KT)}{Kp}\frac{dp}{dt}=0 \tag{28}$$

Here the unburned region, $\psi_f(t)<\psi<1$, is considered to consist of a bulk-gas region, $\psi_f(t)<\psi<\psi_i$, and an end-gas region, $\psi_i<\psi<1$, where ψ_i (given) denotes the interface, or contact surface, between the bulk gas and the end gas. This division of the unburned region holds for $0<t<t_i$. When $t=t_i$, all of the unburned bulk gas has been burned, i.e., $\psi_f(t_i)=\psi_i$. For $t>t_i$, the unburned region consists of just the end-gas region. To distinguish among these regions, the following notation is introduced.

Unburned bulk gas:

$$Y(\psi,t)=Y_u(\psi,t)\qquad T(\psi,t)=T_u(\psi,t),$$
$$\gamma=\kappa\ \text{for}\ \psi_f(t)<\psi<\psi_i \tag{29a}$$

Unburned end gas:

$$Y(\psi,t)=X_u(\psi,t),\quad T(\psi,t)=\Theta_u(\psi,t),$$
$$\gamma=\mu\ \text{for}\ \psi_i<\psi<1 \tag{29b}$$

Burned bulk gas:

$$Y(\psi,t)=Y_b(\psi,t),\quad T(\psi,t)=T_b(\psi,t),$$
$$\gamma=\sigma\ \text{for}\ \psi_i>\psi_f(t)>\psi>0 \tag{29c}$$

Burned end gas:

$$Y(\psi,t)=X_b(\psi,t),\quad T(\psi,t)=\Theta_b(\psi,t),$$
$$\gamma=\Upsilon\ \text{for}\ \psi_f(t)>\psi>\psi_i \tag{29d}$$

For the unburned bulk gas, Eqs. (27) and (28) become

$$\frac{\partial Y_u}{\partial t}=0 \tag{30a}$$

$$\frac{\partial T_u}{\partial t}-\frac{(\kappa-1)}{\kappa}\frac{(1+KT_u)}{Kp}\frac{dp}{dt}=0 \tag{30b}$$

The solutions of Eqs. (30), subject to the initial conditions for this region,

$$p(0)=1,\quad Y_u(\psi,0)=1,\quad T_u(\psi,0)=0,$$

and

$$\psi_f(0)<\psi<\psi_i \tag{31}$$

with $\psi_f(0)=\psi_{f0}\to 0$ and ψ_i constant (to be specified), are

$$Y_u(\psi,t)=1 \tag{32a}$$

$$T_u(\psi,t)=T_u(t)=\frac{1}{K}\{[p(t)]^{(\kappa-1)/\kappa}-1\} \tag{32b}$$

In a similar manner, for the unburned end gas, the solutions of

$$\frac{\partial X_u}{\partial t}=0 \tag{33a}$$

$$\frac{\partial\Theta_u}{\partial t}-\frac{(\mu-1)}{\mu}\frac{(1+K\Theta_u)}{Kp}\frac{dp}{dt}=0 \tag{33b}$$

subject to the initial conditions

$$p(0)=1,\quad X_u(\psi,0)=1,\quad \Theta_u(\psi,0)=0,\ \text{and}\ \psi_i<\psi<1 \tag{34}$$

are

$$X_u(\psi,t)=1 \tag{35a}$$

$$\Theta_u(\psi,t)=\Theta_u(t)=\frac{1}{K}\{[p(t)]^{(\mu-1)/\mu}-1\} \tag{35b}$$

¶On physical grounds, since the pressure is spatially invariant, the results depend on wall *separation* as a function of time; as long as the temporal history of the wall separation is the same, the results are invariant to which (or both) end wall moves. Also, from Eqs. (19) and (22), altering some parameters not only alters the dimensionless groups, but also alters the derived quantity u^*_{u0}, so that the temporal and stream function scales used for nondimensionalization are altered. Thus, for example, altering the value of the activation temperature T^*_a changes the value of β *and* u^*_{u0}, so not only is the value of T at any value of ψ and t (in general) altered, but the associated dimensional quantities ψ^* and t^* are also altered. Finally, in a straightforward generalization of Eq. (24), sparking need not occur necessarily at time $t=0$; e.g., compressional heating owing to the wall motion may occur for a finite time interval before sparking initiates flame propagation.

For the burned bulk-gas region, Eqs. (27) and (28) become

$$\frac{\partial Y_b}{\partial t}=0 \tag{36a}$$

$$\frac{\partial T_b}{\partial t}-\frac{(\sigma-1)}{\sigma}\frac{(1+KT_b)}{Kp}\frac{\mathrm{d}p}{\mathrm{d}t}=0 \tag{36b}$$

The solutions are of the forms

$$Y_b(\psi,t)=H_b(\psi) \tag{37a}$$

$$T_b(\psi,t)=\frac{1}{K}\{F_b(\psi)[p(t)]^{(\sigma-1)/\sigma}-1\} \tag{37b}$$

At the flame,

$$Y_b[\psi_f(t),t]=H_b[\psi_f(t)]:\quad Y_{bf}(t)=H_{bf}(t) \tag{38a}$$

$$T_b[\psi_f(t),t]=\frac{1}{K}\{F_b[\psi_f(t)][p(t)]^{(\sigma-1)/\sigma}-1\}:$$

$$T_{bf}(t)=\frac{1}{K}\{F_{bf}(t)[p(t)]^{(\sigma-1)/\sigma}-1\} \tag{38b}$$

For $t<t_i$ and/or $\psi_f(t)<\psi_i$, the jump conditions at the flame (between the unburned bulk gas and the burned bulk gas) yield

$$Y_{bf}(t)=0\Rightarrow Y_b(\psi,t)=0 \tag{39a}$$

$$T_{bf}(t)=[1+T_u(t)]\Rightarrow F_{bf}(t)=\frac{[p(t)]^{(\kappa-1)/\kappa}+K}{[p(t)]^{(\sigma-1)/\sigma}} \tag{39b}$$

Similarly for $t>t_i$ and/or $\psi_f(t)>\psi_i$,

$$X_b(\psi,t)=0 \tag{40a}$$

$$\Theta_b(\psi,t)=\frac{1}{K}\{G_b(\psi)[p(t)]^{(\Upsilon-1)/\Upsilon}-1\}: \tag{40b}$$

$$\Theta_{bf}(t)=\frac{1}{K}\{G_{bf}(t)[p(t)]^{(\Upsilon-1)/\Upsilon}-1\} \tag{40c}$$

Also,

$$\Theta_{bf}(t)=[1+\Theta_u(t)]\Rightarrow G_{bf}(t)=\frac{[p(t)]^{(\mu-1)/\mu}+K}{[p(t)]^{(\Upsilon-1)/\Upsilon}} \tag{40d}$$

$\psi_f(t)<\psi_i$ (Flame in the Bulk Gas)

For $t<t_i$ and/or $\psi_f(t)<\psi_i$, integration of the mapping equation (21c) over the domain $0\leq\psi\leq 1$ yields

$$\int_0^{L(t)}\mathrm{d}x=\int_0^{\psi_f(t)}\frac{[1+KT_b(\psi,t)]}{p(t)}\mathrm{d}\psi$$

$$+\int_{\psi_f(t)}^{\psi_i}\frac{[1+KT_u(\psi,t)]}{p(t)}\mathrm{d}\psi+\int_{\psi_i}^{1}\frac{[1+K\Theta_u(\psi,t)]}{p(t)}\mathrm{d}\psi:$$

$$L(t)=\frac{1}{[p(t)]^{1/\sigma}}\int_0^{\psi_f(t)}F_b(\psi)\mathrm{d}\psi$$

$$+\frac{[\psi_i-\psi_f(t)]}{[p(t)]^{1/\kappa}}+\frac{(1-\psi_i)}{[p(t)]^{1/\mu}} \tag{41}$$

Upon multiplication by $[p(t)]^{1/\sigma}$, the time derivative of Eq. (41), with rearrangement, produces

$$\frac{1}{\sigma}\frac{p'(t)}{p(t)}\left\{1-\frac{(\kappa-\sigma)}{\kappa}\frac{[\psi_i-\psi_f(t)]}{L(t)[p(t)]^{1/\kappa}}\right.$$

$$\left.-\frac{(\mu-\sigma)}{\mu}\frac{(1-\psi_i)}{L(t)[p(t)]^{1/\mu}}\right\}+\frac{L'(t)}{L(t)}-\frac{K\psi_f'(t)}{L(t)p(t)}=0 \tag{42}$$

Integration of the mapping equation over the unburned domain $\psi<\psi_i<1$, with $\psi\geq\psi_f(t)$, yields

$$\int_{x_u(\psi,t)}^{L(t)}\mathrm{d}x=\int_{\psi}^{\psi_i}\frac{[1+KT_u(\psi_1,t)]}{p(t)}\mathrm{d}\psi_1$$

$$+\int_{\psi_i}^{1}\frac{[1+K\Theta_u(\psi_1,t)]}{p(t)}\mathrm{d}\psi_1:$$

$$x_u(\psi,t)=L(t)-\frac{(\psi_i-\psi)}{[p(t)]^{1/\kappa}}-\frac{(1-\psi_i)}{[p(t)]^{1/\mu}} \tag{43}$$

Note that

$$x_u[\psi_f(t),t]=x_f(t)=L(t)-\frac{[\psi_i-\psi_f(t)]}{[p(t)]^{1/\kappa}}-\frac{(1-\psi_i)}{[p(t)]^{1/\mu}} \tag{44}$$

In turn,

$$\frac{\partial x_u}{\partial t}(\psi,t)=u_u(\psi,t)$$

$$=L'(t)+\frac{p'(t)}{p(t)}\left\{\frac{1}{\kappa}\frac{(\psi_i-\psi)}{[p(t)]^{1/\kappa}}+\frac{1}{\mu}\frac{(1-\psi_i)}{[p(t)]^{1/\mu}}\right\} \tag{45}$$

$$\frac{\mathrm{d}x_f}{\mathrm{d}t}(t)=x_f'(t)=L'(t)+\frac{p'(t)}{p(t)}\left\{\frac{1}{\kappa}\frac{\psi_i-\psi_f(t)}{[p(t)]^{1/\kappa}}\right.$$

$$\left.+\frac{1}{\mu}\frac{(1-\psi_i)}{[p(t)]^{1/\mu}}\right\}+\frac{\psi_f'(t)}{[p(t)]^{1/\kappa}} \tag{46}$$

Thus, the flame speed, the difference between the speed of the flame front and that of the unburned gas at the flame front, is

$$S=S(t)=\left\{x_f'(t)-\lim_{\psi\to\psi_f(t)}[u_u(\psi,t)]\right\}=\frac{\psi_f'(t)}{[p(t)]^{1/\kappa}} \tag{47}$$

In Appendix A, it is determined that, for $\alpha,n=1$ and ν_O, $\nu_F=1$, the flame speed is

$$S(t)\simeq[1+KT_u(t)][1+T_u(t)]^2\exp\{\beta T_u(t)/2[1+T_u(t)]\} \tag{48}$$

It may be shown that $\partial x_u(\psi,t)/\partial t=u_u(\psi,t)$ is continuous at $\psi=\psi_i$, i.e., is continuous across the contact surface between the unburned bulk-gas region and the unburned end-gas region.

Thus, with the motion of the moving wall, i.e., $L(t)$ and $L'(t)$ and the interface location ψ_i specified, the pertinent initial-value problem becomes Eqs. (32b), (35b), (42), (47),

and (48), subject to

$$p(0)=1, \quad T_u(0)=0 \tag{49}**$$

This problem terminates when $t=t_i$, such that

$$p(t_i)=p_i, \ T_u(t_i)=T_{ui}, \ \Theta_u(t_i)=\Theta_{ui}, \ \psi_f(t_i)=\psi_i \tag{50}$$

where p_i, T_{ui}, and Θ_{ui} are found in the course of solution. Here, the motion of the moving wall is approximated as

$$L(t)=\left\{1-\left[\frac{(\mathrm{CR})-1}{2(\mathrm{CR})}\right](1-\cos\omega t)\right\} \tag{51a}$$

$$L'(t)=-\left[\frac{(\mathrm{CR})-1}{2(\mathrm{CR})}\right](\omega\sin\omega t) \tag{51b}$$

where (CR)(>1) is the compression ratio ($L_{\max}/L_{\min}$) $=(1/L_{\min})$ and ω ($=2\pi\Omega=2\pi[\Omega^*/(u^*_{u0}/L^*_0)]$, with Ω^* the number of revolutions per unit time) is the (nondimensional) frequency.

$\psi_f(t)>\psi_i$ (Flame in the End Gas)

For $t>t_i$ and/or $\psi_f(t)>\psi_i$, integration of the mapping equation (21c) over the domain $0\leq\psi\leq 1$ yields

$$L(t)=\frac{1}{[p(t)]^{1/\sigma}}\int_0^{\psi_i}F_b(\psi)\mathrm{d}\psi + \frac{1}{[p(t)]^{1/\Upsilon}}\int_{\psi_i}^{\psi_f(t)}G_b(\psi)\mathrm{d}\psi+\frac{[1-\psi_f(t)]}{[p(t)]^{1/\mu}} \tag{52}$$

Thus, for this case,

$$\frac{1}{\sigma}\frac{p'(t)}{p(t)}\left\{1-\frac{(\mu-\sigma)}{\mu}\frac{[1-\psi_f(t)]}{L(t)[p(t)]^{1/\mu}}-\frac{(\Upsilon-\sigma)}{\Upsilon}\times\left[\int_{\psi_i}^{\psi_f(t)}G_b(\psi)\mathrm{d}\psi\Big/L(t)[p(t)]^{1/\Upsilon}\right]\right\} + \frac{L'(t)}{L(t)}-\frac{K\psi_f'(t)}{L(t)p(t)}=0 \tag{53}$$

where it is approximated that

$$\int_{\psi_i}^{\psi_f(t)}G_b(\psi)\mathrm{d}\psi\simeq\frac{[\psi_f(t)-\psi_i]}{2}\{G_b[\psi_f(t)]+G_b(\psi_i)\} \tag{54a}$$

$$G_b[\psi_f(t)]=\frac{[p(t)]^{(\mu-1)/\mu}+K}{[p(t)]^{(\Upsilon-1)/\Upsilon}}, \quad G_b(\psi_i)=\frac{p_i^{(\mu-1)/\mu}+K}{p_i^{(\Upsilon-1)/\Upsilon}} \tag{54b}$$

**From Eqs. (42) and (49) for $L'=0$, $\kappa=\sigma$, and $\psi_i=1$, one recovers the following classical results, if $p=p_1$ when $\psi_f=1$:

$$p(t)-1=\sigma K\psi_f(t)\Rightarrow p_1-1=\sigma K\Rightarrow\frac{p(t)-1}{p_1-1}=\psi_f(t)$$

This implies that the peak value of T_u is

$$(T_u)_{\max}=\frac{1}{K}\{[1+\sigma K]^{(\sigma-1)/\sigma}-1\}$$

Integration of the mapping equation over the (end-gas) unburned domain $\psi<1$, with $\psi\geq\psi_f(t)$, yields

$$x_u(\psi,t)=L(t)-\frac{(1-\psi)}{[p(t)]^{1/\mu}} \tag{55a}$$

$$x_u(\psi_f(t),t)=x_f(t)=L(t)-\frac{[1-\psi_f(t)]}{[p(t)]^{1/\mu}} \tag{55b}$$

In turn,

$$\frac{\partial x_u}{\partial t}(\psi,t)=u_u(\psi,t)=L'(t)+\frac{p'(t)}{p(t)}\left\{\frac{1}{\mu}\frac{(1-\psi)}{[p(t)]^{1/\mu}}\right\}$$

$$\frac{\mathrm{d}x_f}{\mathrm{d}t}(t)=x_f'(t)$$

$$=L'(t)+\frac{p'(t)}{p(t)}\left\{\frac{1}{\mu}\frac{[1-\psi_f(t)]}{[p(t)]^{1/\mu}}\right\}+\frac{\psi_f'(t)}{[p(t)]^{1/\mu}} \tag{56}$$

Thus, the flame speed is

$$S=S(t)=\left\{x_f'(t)-\lim_{\psi\to\psi_f(t)}[u_u(\psi,t)]\right\}=\frac{\psi_f'(t)}{[p(t)]^{1/\mu}} \tag{57}$$

where, for α, $n=1$ and ν_O, $\nu_F=1$,

$$S(t)\simeq[1+K\Theta_u(t)][1+\Theta_u(t)]^2\times\exp\{\beta\Theta_u(t)/2[1+\Theta_u(t)]\} \tag{58}$$

Thus, for this domain, the pertinent initial-value problem is given by Eqs. (35b), (53), (54), (57), and (58), where

$$p(t_i)=p_i, \quad \Theta_u(t_i)=\Theta_{ui}, \quad \psi_f(t_i)=\psi_i \tag{59}$$

The problem nominally terminates when $t=t_1$, such that

$$p(t_1)=p_1, \quad \Theta_u(t_1)=\Theta_{u1}, \quad \psi_f(t_1)=1 \tag{60}$$

The above generalization of earlier, variable-volume enclosure work[7] entails a flame speed that is derived from the adopted reaction rate (cf., Ref. 8) and reduces to the laminar isobaric value as $t\to 0$ (cf., Ref. 9).

IV. Discussion

First, in Appendix B it is shown that for the circumstances of interest, heat transfer (to slippery noncatalytic side walls) may be simulated conveniently by assignment of values to the polytropic constants κ, μ, σ, and Υ, i.e., the polytropic constants are effectively equivalent to the introduction of heat-transfer coefficients: the smaller the value assigned to a polytropic constant, the greater the heat transfer in the associated domain. While adequate experimental identification of polytropic constants (or heat-transfer coefficients) seems yet to be reported in the literature, the consequences of assigning relative values permits the comparison of heat-transfer requirements for varying parametric conditions.

Second, in singular-perturbation terms, end-gas knock is the physical manifestation of the possible nonuniform validity in time of the asymptotic approximation (based on $\beta\gg 1$) that the reaction rate contribution is negligible in the unburned gas; however, the asymptotic approximation (based on $\epsilon\ll 1$) that the diffusion contribution is negligible remains uniformly valid. Thus, retaining the chemical reaction terms in Eq. (16) that were discarded in writing Eqs. (27) and (28) because the terms were taken to be exponentially small, one

has

$$\frac{\partial Y}{\partial t} = -\frac{1}{\epsilon}\Lambda_0 pY(1+\Phi Y)\exp[-\beta(1-T)/T] \quad (61)$$

$$\frac{\partial T}{\partial t} = \frac{1}{\epsilon}\Lambda_0 pY(1+\Phi Y)\exp[-\beta(1-T)/T] + \frac{(\gamma-1)}{\gamma}\frac{(1+KT)}{Kp}\frac{dp}{dt} \quad (62)$$

where $[Y(\psi,t),\ T(\psi,t),\ \gamma] \rightarrow [Y_u(t),\ T_u(t),\ \kappa]$ in the unburned bulk-gas region and $[Y(\psi,t),\ T(\psi,t),\ \gamma] \rightarrow [X_u(t),\ \Theta_u(t),\ \mu]$ in the unburned end-gas region. It is recalled that adjustment of the polytropic constant γ simulates the effect of heat loss. Subject to the initial conditions $Y(0)=1$ and $T(0)=0$, this is a variant to the classical spatially homogeneous, nonstationary ignition problem in which the criterion for an explosion self-sustained against heat loss is sought. Here, compressional heating, as reflected in the pressure $p(t)$, raises the temperature of the premixture; clearly, as T rises in time, the reaction rate term may become comparable to the other terms in the energy equation. If one substitutes the pressure $p(t)$ from solution of the problem posed in Sec. III, then one can obtain an indication from Eqs. (61) and (62) whether significant autoconversion occurs in the end gas prior to the completion of flame propagation. If modest autoconversion causes a pressure rise in time during the flame transit beyond that accounted for in the theory of Sec. III,[9] that development is not easily generalized to include it.[4] Of more concern is the very significant autoconversion of the unburned gas on a time scale comparable to, or less than, the time scale for the completion of flame propagation. Especially if the time scale is less than that for completion of flame propagation (and less than that for acoustic adjustment), there occurs effectively a constant-volume explosion of the unburned gas. Such a relatively instantaneous reaction of unburned gas results in a pressure in the end-gas region higher than that in the rest of the gas. The consequence is nonlinear pressure waves and an audible sound from the sympathetic vibration of the engine components. However, there is no incentive to pursue the solution into this spatially nonuniform pressure domain because the above formulation is inadequate.

The standard asymptotic solution for $\beta \gg 1$ of Eqs. (61) and (62), or even of Eq. (62) with the reactant consumption ignored (i.e., $Y \equiv 1$), suffices to establish that, for plausible parameter assignments for hydrocarbon-air premixtures of automotive interest, autoconversion becomes effectively instantaneous relative to the flame propagation speed over (say) a half centimeter for unburned gas temperatures on the order of 1025 K.[4] Practical experimental data for nonisobaric combustion also give this value.[1] Mathematical treatment beyond that in Appendix C seems to be of limited engineering utility.

Thus, the following computational procedure is evolved to answer the questions posed in the last paragraph of Sec. I. First, with κ and σ taken as given and ψ_i set equal to unity (so there is no end gas), the first initial-value problem posed in Sec. III is carried out for the parametric assignments of interest. If it holds uniformly in time that the temperature of the unburned gas $T_u^* < 1025$ K (for specificity), then knock is taken not to occur. If, however, T_u^* reaches 1025 K for $\psi_f(t) < 1$, then that value of ψ_f is taken as ψ_i, i.e., ψ_i is the fraction of the charge identified as bulk gas and $(1-\psi_i)$ as end gas. Then, with Υ taken as given, the largest value of μ for which $\Theta_u^* \rightarrow 1025$ K as $\psi_f \rightarrow 1$ is sought by trial and error. That is, the minimal amount of heat transfer from the end gas is sought such that significant end-gas autoconversion is barely precluded. In this manner, the fraction (if any) of the charge that would undergo rapid autoconversion is identified and the relative heat-transfer provision to preclude such autoconversion is determined.

In the present formulation, with adiabatic end walls, heat transfer is effected through the (noncatalytic slippery) side walls. Incorporation of finite heat transfer through the end walls would necessitate the introduction of thermally diffusive layers in the vicinity of $\psi = 0,1$; while such boundary layers would thicken in time, they would remain thin relative to the flow domain length for the time span and the parametric assignments of interest ($\epsilon \ll 1$). Such end wall quench layers have been examined in other contexts; their introduction in the present context would seem to incur nonessential complication, such as end gas in a nonuniform thermodynamic state. The only precaution (already noted) is that very excessive heat transfer from the end gas could so retard flame propagation that expansional cooling (from the piston motion) would leave a residual unburned premixture on the time scales of practical interest.

V. Computational Examples

A limited number of examples now are presented of the procedure discussed in the penultimate paragraph of Sec. IV. For brevity of reference, the following assignment of (mainly) dimensional parameters is termed nominal:

$$T_{u0}^* = 300 \text{ K},\ T_{b0}^* = 1800 \text{ K},\ T_a^* = 15{,}000 \text{ K},\ \phi = 0.8,$$

$$D_{u0}^* = 0.1 \text{ cm}^2/\text{s},\ u_{u0}^* = 40 \text{ cm/s},\ L_0^* = 10 \text{ cm},\ Le = 1,$$

$$\Omega^* = 20 \text{ rev/s} \quad (63)$$

It is consistent with these assignments to adopt the following "nominal" values for the dimensionless parameters (the parameter ϵ does not enter the calculations—its value is given only for completeness):

$$\beta = 10,\ \Lambda_0 = 50,\ K = 5,\ \Phi = 4,\ \epsilon = 2\times 10^{-4},\ \omega \doteq 31.4,$$

$$\mu = 1.4,\ \kappa = 1.4,\ \Upsilon = 1.4,\ \sigma = 1.4,\ \text{CR} = 6,\ \theta_{ig} = 135 \text{ deg} \quad (64)$$

The last assignment, alluded to earlier in the footnote to Eq. (25b) implicitly gives the time of sparking or, more precisely, the time at which flame propagation commences. That is, it is defined that

$$\theta = \omega t \quad (65)$$

so at the beginning of compression $t=0$, it holds that $\theta = 0$, which corresponds to "bottom dead center" [$L=1$, the maximum value of L, from Eq. (51a)]. At $\theta = \theta_{ig}$ (assigned, i.e., at $t_{ig} = \theta_{ig}/\omega$) the variables $\psi_f(t)$ and $x_f(t)$, held at zero for $0 < t < t_{ig}$, take on values consistent with Eqs. (47) and (44). While sparking and compression could commence simultaneously so that $t_{ig} = \theta_{ig} = 0$, sparking occurs, in general, after a finite interval of compression so $t_{ig} > 0$. In the nominal case, $\theta_{ig} = 135$ deg or flame propagation commences after about 6/7ths of the length of the (compressional) stroke. All of the parameters are held at their nominal values through the computations unless explicitly stated otherwise.

The onset of knock is taken to occur at $T_u = 0.4$ or, from Eq. (63), at a temperature of 900 K—a value slightly lower than that cited elsewhere in this paper.

The nominal case is found (by design) to be just barely knock free. Computation indicates that combustion is completed at $t \doteq 0.088$; since the basis of nondimensionalization is $L_0^*/u_{u0}^* = 0.25$ s, combustion lasts 22 ms or about three-to-four times longer than in a typical Otto cycle automotive engine. At the completion of burning, $T_u \doteq 0.399$, $p \doteq 46.6$, $\theta = 157$ deg, and $L = 0.197$, whereas at the start of burning, $t = 0.075$, $T_u = 0.129$, $p = 5.69$, and $L = 0.289$. As with all of the cases to be examined, combustion is completed during

the compression stroke, i.e., at crank angle $\theta < 180$ deg. Of course, in an automotive context, the combustion interval is likely to be (very roughly) symmetric with respect to the time of the piston position at top center.

If the polytropic constant of the burned gas σ is reduced in value from 1.4 to 1.1, all other parameters being held fixed, then at the completion of burning $t = 0.089$, $T_u = 0.378$, $p = 40.945$, $\theta = 159.8$ deg, and $L = 0.192$, whereas at the start of burning the corresponding values are (of course) those given in the preceding paragraph. Since modifying the heat transfer from the burned gas is seen to have but modest effect on the temperature of the unburned gas, this parametric variation is not pursued further here.

Table 1 presents results for four parametric variations, all selected to incur knock. The heat-transfer requirement from the end gas that precludes knock is identified in the form of the maximum value of μ (denoted μ_{crit}) that still permits $\Theta_u < 0.4$ at all times during the combustion event. Further results for the case CR = 12 are presented in Figs. 1-3 and for the case $K = 3$ in Figs. 4-6. The other two variations examined are $\theta_{ig} = 165$ deg and $\omega = 51.6$. These cases entail between 13 and 57% of the initial combustible mass being involved in autoconversion (in the absence of augmented end-gas heat transfer) and, in this sense, represent a spectrum of cases. In Figs. 2, 3, 5, and 6 it may be recalled that $x_i(t)$, the inter-

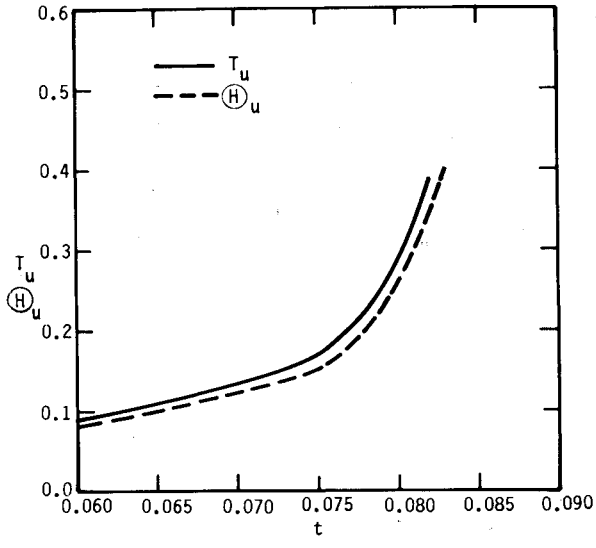

Fig. 1 For nominal parametric assignments, defined by Eqs. (63-65), except that the compression ratio CR = 12, the dimensionless unburned bulk-gas temperature T_u and the dimensionless unburned end-gas temperature Θ_u are presented as functions of dimensionless time t, where compression commences at $t = 0$. When the flame enters the end gas, T_u is no longer defined. Here, the scale for nondimensionalization of time is 22 ms; $T = 0$ corresponds to 300 K, $T = 0.2$ to 600 K, $T = 0.4$ to 900 K. Augmented heat transfer from an appropriate portion of the mixture, the last-to-burn charge (end gas), precludes any unburned gas achieving a rapid-autoconversion-precipitating temperature, taken as 900 K.

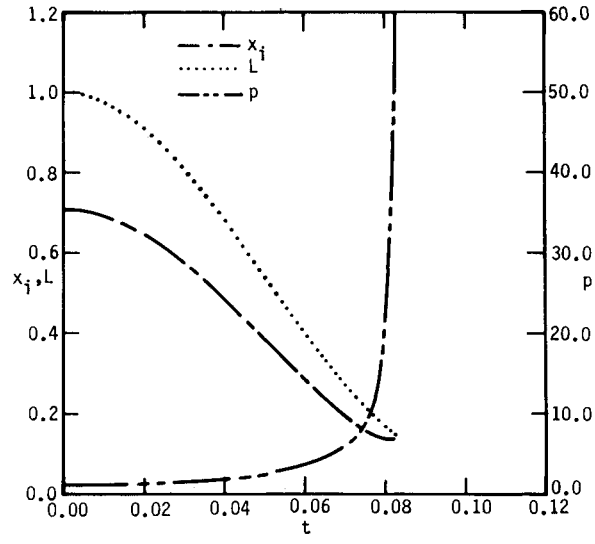

Fig. 2 For case of Fig. 1, the dimensionless dependent variables pressure p, combustion-chamber length L, and interface position x_i between unburned bulk gas and unburned end gas are presented as functions of dimensionless time t. When flame enters end gas, x_i is no longer defined. Pressure is nondimensionalized against its initial value, here 1 atm, and lengths are nondimensionalized against initial chamber length, here 10 cm.

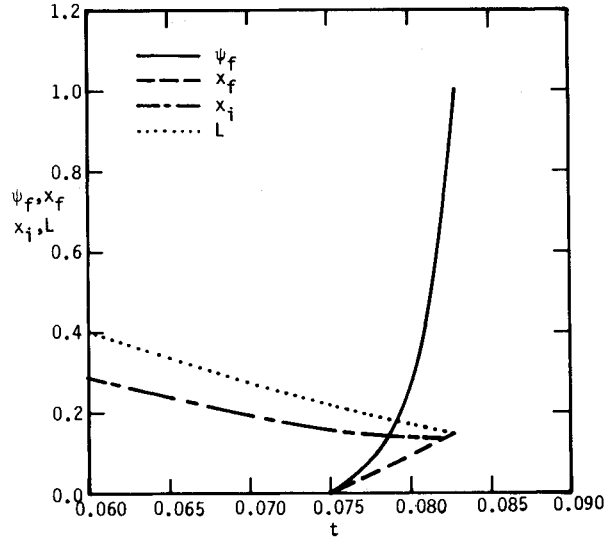

Fig. 3 For case of Fig. 1, dimensionless dependent variables chamber length L, interface position x_i between unburned bulk gas and unburned end gas, flame position x_f, and fraction ψ_f of total initial premixture burned, are presented as functions of time t. The length x_f, like x_i, is nondimensionalized against initial chamber length, here 10 cm.

Table 1 Parametric variations on the nominal (threshold-knock) case[a]

	Flame enters end gas ($\psi_f = \psi_i$)							Flame propagation complete ($\psi_f = 1$)				
Case	t	θ, deg	L	x_f	ψ_f	p	Θ_u	t	θ, deg	L	p	μ_{crit}
CR = 12	0.082	147.6	0.16	0.13	0.71	45.6	0.35	0.083	149.1	0.15	63.0	1.3604
$K = 3$	0.083	150.5	0.22	0.14	0.41	15.7	0.30	0.088	157.8	0.20	30.3	1.3002
$\omega = 51.6$	0.056	166.4	0.18	0.17	0.87	45.6	0.38	0.057	167.7	0.18	52.6	1.3836
$\theta_{ig} = 165$ deg	0.098	77.0	0.17	0.16	0.83	46.2	0.37	0.099	177.9	0.17	54.3	1.3795

[a]For the case $K = 3$, if $p_0^* = 1$ atm, since $T_{u0}^* = 450$ K, then the initial density ρ_{u0}^* is reduced to two-thirds that of the other cases.

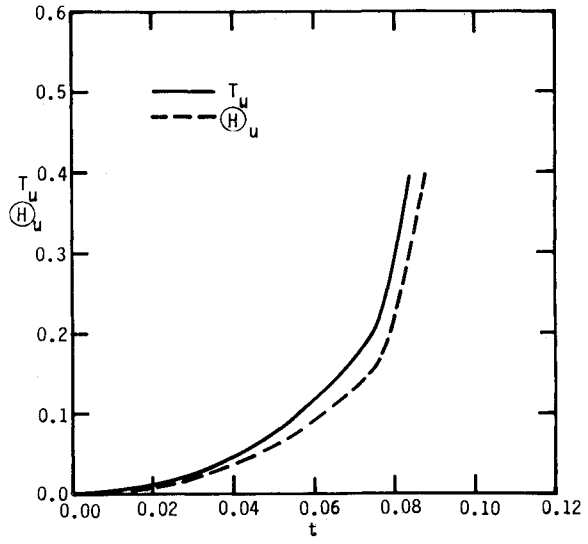

Fig. 4 For the nominal parametric assignments defined by Eqs. (63-65), except that the ratio of chemical exothermicity to initial enthalpy $K=3$, dimensionless temperature T_u, and dimensionless unburned end-gas temperature Θ_u, are presented as functions of time t. The scale for nondimensionalization of time is 22 ms; $T=0$ corresponds to 300 K, $T=0.2$ to 620 K, $T=0.4$ to 990 K (taken as the rapid-autoconversion temperature to be avoided by augmented heat transfer from the end gas).

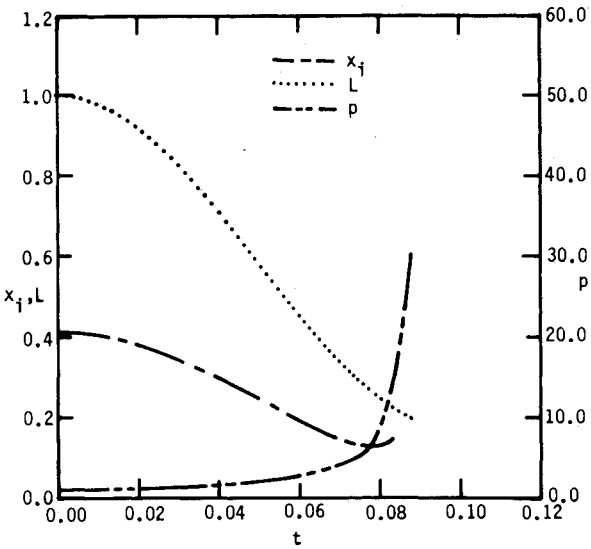

Fig. 5 For the case of Fig. 4, a presentation exactly analogous to that of Fig. 2.

face between the unburned end gas and the unburned bulk gas, is not defined for $x_f(t)>x_i(t)$ and accordingly is neither computed nor plotted. It may be noted that the larger the fraction of end gas (i.e., the smaller the value of ψ_i), the larger the heat-transfer requirement to preclude knock (i.e., the smaller the value of μ_{crit}). However, it is noteworthy that reduction of K (from its nominal value of 5) to 3, while β is held constant, implies T_u^* is altered from 300 to 450 K. Since $T_u=0.4$ is retained as a knock criterion, $T^*=990$ K becomes the temperature for explosive conversion of the reactant to the product gas.

As a cautionary note concerning other parameteric variations, it may be noted, for example, that if Y_{Fu} is altered, then ϕ and T_{b0}^* are altered, from the discussion following

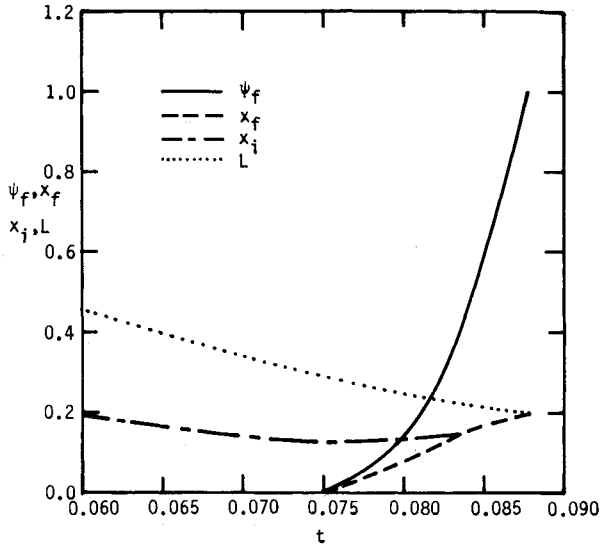

Fig. 6 For the case of Fig. 4, a presentation exactly analogous to that of Fig. 3.

Eq. (15). Hence, β, Λ_0, and K are altered from Eqs. (19) and (22), but also u_{u0}^* (utilized in the nondimensionalization of time t^* and the piston speed parameter Ω^*) is altered from Eq. (19).

VI. Conclusions

The present development has concentrated on enhancing heat transfer as a countermeasure to end-gas knock. Another (perhaps complementary) strategy is to seek fuel additives that inhibit end-gas autoconversion without impeding flame propagation. While trial-and-error testing yielded the knock-inhibiting fuel additives of the past (such as tetraethyl lead, now constrained from use because it poisons exhaust-gas-treating catalysts), it remains to be seen whether retention[11] of detailed chemical kinetic rates and mechanisms for fuels of practical interest can assist identification of a substitute, environmentally acceptable knock-inhibiting additive.††

Appendix A: Flame Zone Structure

As in the unbounded (isobaric) case, the structure of the flame zone for the bounded (nonisobaric, enclosed) case for $\epsilon \ll 1$, with $\beta \gg 1$, consists of a convective-diffusive region and a diffusive-reactive region. The results presented are for α, $n=1$ and ν_F, $\nu_O=1$.

††The evolution of a planar flame propagating through a "not too far from stoichiometric" premixture enclosed in a sufficiently long constant-volume duct to a so-called tulip[12,13] shape may be evidence of a "miniknock" event.[14] It is observed that such a flame ultimately propagates less rapidly in a duct at midheight (relative to near-ceiling and near-floor flame positions). Although the temperature in the compressionally heated unburned gas may not exceed about 600 K in such tests, perhaps cool-flame (and possibly other subsequent, modestly exothermic, low-temperature) reactions engender enough end-gas counterflow to the deflagration wave speed that flame progression is retarded at duct midheight. Presumably, friction inhibits the counterflow near ceiling and floor, so the flame locally propagates relatively unimpeded. Incidentally, for long enough tubes, or for tubes of a small enough cross section, spatial gradients of pressure plausibly arise such that the effect of the tulip flame shape could be observed even if the extremity of the tube near the burned (or even unburned) premixture were open to the atmosphere.[12] Since the end-gas temperatures are typically over 1000 K for knock, the significance of cool-flame (and possibly other subsequent low-temperature) reactions in rapid-compression machines under knocking conditions is unclear.

For the convective-diffusive region, the appropriate transformation of variables is $(\psi,t)\rightarrow(\xi,t)$, where

$$\xi(\psi,t;\ldots)=M(t)E(t;\beta)\{[\psi_f(t)-\psi]/\epsilon\} \tag{A1}$$

The domain of this region is $-\infty<\xi<0$, $t>0$, such that the unburned exterior region is approached as $\xi\rightarrow\infty$. Further, the flame speed is taken to be

$$S(t;\ldots)=\psi_f'(t;..)/[p(t)]^{1/\kappa}\simeq V(t)E(t,\beta)[1+\mathcal{O}(\beta^{-1})] \tag{A2}$$

Here,

$$E(t;\beta)=\exp\{\beta[T_b(t)-1]/2T_b(t)\}$$

$$=\exp\{\beta T_u(t)/2[1+T_u(t)]\} \tag{A3}$$

$$M(t)=[T_b(t)]^2=[1+T_u(t)]^2 \tag{A4a}$$

$$V(t)=[p(t)]^{(\kappa-1)/\kappa}[T_b(t)]^2$$

$$=[1+KT_u(t)][1+T_u(t)]^2 \tag{A4b}$$

Note that $\xi\rightarrow(-\psi)/\epsilon$ and $S\rightarrow 1$ as $t\rightarrow 0$, such that the unbounded case is the initial condition of the bounded case. Through the matching of the solutions of this convective-diffusive region with those of the diffusive-reactive region it is demonstrated that Eq. (A2) is the correct asymptotic representation of the flame speed.

For this region, the dependent variables are of the forms

$$Y(\psi,t;\ldots)\simeq X(\xi,t;\ldots)[1+\mathcal{O}(\beta^{-1})] \tag{A5a}$$

$$T(\psi,t;\ldots)\simeq F(\xi,t;\ldots)[1+\mathcal{O}(\beta^{-1})] \tag{A5b}$$

Thus, for these scalings, the specific time derivative terms and the reaction rate terms can be neglected, such that, to leading order of approximation, Eqs. (16) and (17) become

$$\frac{\partial^2 X}{\partial\xi^2}-\frac{\partial X}{\partial\xi}=0 \tag{A6}$$

$$Le\frac{\partial^2 F}{\partial\xi^2}-\frac{\partial F}{\partial\xi}=0 \tag{A7}$$

The boundary conditions for these equations are

$$X\rightarrow 1,\quad F\rightarrow T_u \text{ as } \xi\rightarrow-\infty \tag{A8a}$$

$$X\rightarrow 0,\quad F\rightarrow T_{bf}=(1+T_u) \text{ as } \xi\rightarrow 0 \tag{A8b}$$

The solutions of these convective-diffusive region boundary value problems are

$$X(\xi,t)=[1-\exp(\xi)] \tag{A9}$$

$$F(\xi,t)=[T_u(t)+\exp(\xi/Le)]=T_{bf}(t)-[1-\exp(\xi/Le)] \tag{A10}$$

It is seen that

$$X\rightarrow 1,\ F\rightarrow T_u(\text{exponentially}) \text{ as } \xi\rightarrow-\infty \tag{A11}$$

and that

$$X\sim-\xi(1+\ldots)\rightarrow 0+ \tag{A12a}$$

$$F\sim T_b+(\xi/Le)(1+\ldots)\rightarrow T_b \text{ as } \xi\rightarrow 0- \tag{A12b}$$

For the diffusive-reaction region, the transformation of variables is $(\psi,t)\rightarrow(\eta,t)$, where

$$\eta(\psi,t;\ldots)=E(t;\beta)\{[\psi_f(t)-\psi]/\beta^{-1}\epsilon\} \tag{A13}$$

where $E(t;\beta)$ is given in Eq. (A3). The domain of this region is $-\infty<\eta<\infty$, $t>0$, such that the burned exterior region is approached as $\eta\rightarrow\infty$. The flame speed is still that given in Eq. (A2) et seq. Again, note that, as $t\rightarrow 0$, $\eta\rightarrow(-\psi)/\beta^{-1}\epsilon$ and $S\rightarrow 1$.

For this region, the dependent variables are taken to be

$$Y(\psi,t;\ldots)\simeq\beta^{-1}[T_b(t)]^2Z(\eta,t;\ldots)[1+\mathcal{O}(\beta^{-1})]$$

$$=\beta^{-1}[1+T_u(t)]^2Z(\eta,t;\ldots)[1+\mathcal{O}(\beta^{-1})] \tag{A14a}$$

$$T(\psi,t;\ldots)\simeq T_b(t)-\beta^{-1}[T_b(t)]^2G(\eta,t;\ldots)[1+\mathcal{O}(\beta^{-1})]$$

$$=[1+T_u(t)]-\beta^{-1}[1+T_u(t)]^2G(\eta,t;\ldots)[1+\mathcal{O}(\beta^{-1})] \tag{A14b}$$

For $\epsilon\ll 1$ and $\beta\gg 1$, under these scalings to leading order of approximation for this region, the convective terms can be neglected and Eqs. (16) and (17) become

$$\frac{\partial^2 Z}{\partial\eta^2}=\frac{1}{2Le^2}Z\exp(-G) \tag{A15}$$

$$Le\frac{\partial^2 G}{\partial\eta^2}=\frac{1}{2Le^2}Z\exp(-G) \tag{A16}$$

The boundary conditions are

$$Z,G\rightarrow 0 \text{ as } \eta\rightarrow\infty \tag{A17a}$$

$$Z,G\rightarrow\infty \text{ as } \eta\rightarrow-\infty \tag{A17b}$$

By subtracting Eq. (A16) from Eq. (A15) and by using Eq. (A17), $Z=LeG$. Then Eqs. (A15-A17) reduce to

$$\frac{\partial^2 G}{\partial\eta^2}=\frac{1}{2Le^2}G\exp(-G) \tag{A18a}$$

$$G\rightarrow 0 \text{ as } \eta\rightarrow\infty,\quad G\rightarrow\infty \text{ as } \eta\rightarrow-\infty \tag{A18b}$$

The first integral of this equation is

$$\frac{\partial G}{\partial\eta}=-\frac{1}{Le}[1-(1+G)\exp(-G)]^{1/2} \tag{A19}$$

Thus, it is determined that

$$G\sim[\exp(-\eta/2^{1/2}Le)](1+\ldots)\rightarrow 0 \text{ as } \eta\rightarrow\infty \tag{A20a}$$

$$G\sim-(\eta/Le)(1+\ldots) \text{ as } \eta\rightarrow-\infty \tag{A20b}$$

Upon returning to the original dependent variables, it is seen that, for the solutions of the convective-diffusive and diffusive-reactive regions,

$$Y\sim[(-\xi)+\ldots]+\ldots \text{ as } \xi\rightarrow 0-$$

$$Y\sim\beta^{-1}\{(1+T_u)^2[(-\eta)+\ldots]\}+\ldots \text{ as } \eta\rightarrow-\infty \tag{A21a}$$

$$T\sim[(1+T_u)-(-\xi/Le)+\ldots]+\ldots \text{ as } \xi\rightarrow 0-$$

$$T\sim(1+T_u)-\beta^{-1}\{(1+T_u)^2$$

$$\times[(-\eta/Le)+\ldots]\}+\ldots \text{ as } \eta\rightarrow-\infty \tag{A21b}$$

Since $\eta=\beta\xi/(1+T_u)^2$, the solutions match for these two regions, which involved the specification of the leading-order approximation of the flame speed. In the text, this flame speed is expressed as

$$S(t)\simeq S(T_u(t);\beta,K)=[1+KT_u(t)][1+T_u(t)]^2 \times\exp\{\beta T_u(t)/2[1+T_u(t)]\} \tag{A22}$$

Appendix B: Polytropic Law to Simulate Heat Transfer during the Combustion Event in an Enclosure

If the use of a super asterisk to denote a dimensional quantity is dispensed with in this Appendix, then, in conventional notation from thermodynamics,

$$c_v\frac{dT}{dt}+p\frac{d(1/\rho)}{dt}=q \tag{B1}$$

where q denotes the rate of heat addition per unit mass in the enclosure. Hence, for an ideal gas,

$$\frac{d(\ell nT)}{dt}-(\gamma-1)\frac{d(\ell n\rho)}{dt}=\frac{d(\ell np)}{dt}-\gamma\frac{d(\ell n\rho)}{dt}=\frac{q}{c_vT} \tag{B2}$$

For tractability, let $q=-\epsilon c_vT$, with the constant $\epsilon>0$; the product ϵc_v plays the role of a heat-transfer coefficient. Then, if subscript 0 denotes the initial state,

$$\frac{d}{dt}\left[\ell n\left(\frac{p}{\rho^\gamma}\right)\right]=-\epsilon\Rightarrow\frac{p}{\rho^\gamma}=\frac{p_0}{{\rho_0}^\gamma}\exp(-\epsilon t) \tag{B3}$$

During combustion, as a rough approximation, if the constant $\mu>0$, with μ distinct from that of Eq. (29b),

$$\frac{p}{p_0}\doteq\exp(\mu t)\Rightarrow\frac{1}{\mu}\ell n\left(\frac{p}{p_0}\right)=t \tag{B4}$$

Hence, substitution for t by means of Eq. (B4) gives

$$\exp(-\epsilon t)=\exp\left[-\frac{\epsilon}{\mu}\ell n\left(\frac{p}{p_0}\right)\right]=\left(\frac{p}{p_0}\right)^{-\epsilon/\mu} \tag{B5}$$

Use of Eq. (B5) in Eq. (B3) gives

$$\left(\frac{p}{p_0}\right)^{1+(\epsilon/\mu)}=\left(\frac{\rho}{\rho_0}\right)^\gamma\Rightarrow\frac{\rho}{\rho_0}=\left(\frac{p}{p_0}\right)^{1/\gamma_*}$$

$$\frac{1}{\gamma_*}=\frac{1}{\gamma}\left(1+\frac{\epsilon}{\mu}\right) \tag{B6}$$

Since $(\epsilon/\mu)>0$, $\gamma>\gamma_*$. That is, the effect of the heat transfer from a flow with rising pressure may be simulated by adoption of the polytropic constant reduced from the adiabatic value. Furthermore, via Eq. (B6), the polytropic constant may be related to the heat-transfer coefficient (and a characterization of the rate of pressure rise).

Appendix C: Autoconversion Criterion

In Eqs. (16-22), with $\epsilon\ll1$ and $\beta\gg1$, it is anticipated that a physically interesting, autoconversion-related case entails the following quantitative relation between the values of the (more generally, independent) parameters ϵ, β:

$$\epsilon\equiv\beta^2\exp(-\beta T_\epsilon),\ \text{with}\ T_\epsilon=\mathcal{O}(1) \tag{C1}$$

It is convenient to introduce the notation

$$\Theta_\epsilon\equiv(1+T_\epsilon)^{-1}<1\Rightarrow T_\epsilon=(1-\Theta_\epsilon)/\Theta_\epsilon$$

$$\beta_\epsilon=(1+T_\epsilon)\beta>\beta \tag{C2}$$

Hence, from Eqs. (C1) and (C2),

$$\epsilon=\beta_\epsilon^2\Theta_\epsilon^2\exp[-\beta_\epsilon(1-\Theta_\epsilon)] \tag{C3}$$

The subscript ϵ denotes conditions at which it is anticipated that chemical conversion may no longer be neglected in the end gas, although the diffusive transfer remains negligible. This statement may be more readily noted by rewriting Eqs. (16) and (17) under Eqs. (C1-C3) as

$$\frac{\partial Y}{\partial t}\simeq-\frac{1}{2Le^2}pY(1+\Phi Y)\exp[-\beta_\epsilon(\Theta_\epsilon-T)/T] \tag{C4}$$

$$\frac{\partial T}{\partial t}\simeq\frac{1}{2Le^2}pY(1+\Phi Y)\exp[-\beta_\epsilon(\Theta_\epsilon-T)/T] +\frac{\gamma-1}{\gamma}\frac{(1+KT)}{Kp}\frac{dp}{dt} \tag{C5}$$

For $0\lesssim T\lesssim\Theta_\epsilon$, the reaction term is negligible; this interval is also characterized by the following:

$$0<t<\tau_\epsilon,\quad 1<p<\Pi_\epsilon \tag{C6}$$

where the definitions of the constants τ_ϵ and Π_ϵ are evident. Within this interval, solution is given by Eqs. (32), in the unburned bulk gas and by Eqs. (35) in the unburned end gas. For the typical values $\epsilon\simeq2\times10^{-4}$ and $\beta\simeq10$, Eq. (C1) gives $T_\epsilon\simeq1.31$, $\Theta_\epsilon\simeq0.432$, and $\beta_\epsilon\simeq23.1$; for $\epsilon\simeq2\times10^{-4}$ but $\beta\simeq5$ (a somewhat small value), $T_\epsilon\simeq2.35$, $\Theta_\epsilon\simeq0.299$, and $\beta_\epsilon\simeq16.8$. From Eq. (13), if $T^*_{u0}\simeq300$ K and $T^*_{b0}\simeq2100$ K, the condition $T=\Theta_\epsilon$ implies $T^*\simeq1078$ K for $\beta\simeq10$ and $T^*\simeq840$ K for $\beta\simeq5$. The value for T^* used in the text is on the order of $\Theta_\epsilon\simeq0.4$, or $T^*\simeq1025$ K.

Equations (C4) and (C5) may be brought into the classical canonical form for study of the transition to explosion by introduction of the following expansion about the state ϵ:

$$\tau=\beta_\epsilon\frac{(1+\Phi)(\Pi_\epsilon/\Theta_\epsilon)}{2Le^2}(t-\tau_\epsilon),\quad Y=1-\beta_\epsilon^{-1}\Theta_\epsilon X \tag{C7}$$

$$T=\Theta_\epsilon(1+\beta_\epsilon^{-1}\Theta),\quad p=\Pi_\epsilon(1+\beta_\epsilon^{-1}\Pi) \tag{C8}$$

Substitution of Eqs. (C7) and (C8) into Eqs. (C4) and (C5) yields to leading order,

$$\frac{\partial X}{\partial\tau}\simeq\exp(\Theta) \tag{C9a}$$

$$\frac{\partial\Theta}{\partial\tau}\simeq\exp(\Theta)+\frac{(\gamma-1)}{\gamma}\frac{(1+K\Theta_\epsilon)}{K\Theta_\epsilon}\frac{d\Pi}{d\tau} \tag{C9b}$$

where

$$X=\Theta-\frac{(\gamma-1)}{\gamma}\frac{(1+K\Theta_\epsilon)}{K\Theta_\epsilon}\Pi \tag{C10}$$

is an integral. To the lowest order at the outset of the transition, reactant depletion need not be accounted for in the heat balance. Also, it is recalled that adjustment of the value of γ is taken as a convenient alternative to the introduction

of a heat-transfer coefficient for incorporating thermal loss effects during a process in which the pressure rises in time.‡‡

Incidentally, from Eqs. (C1), (C2), and (C8) for a long enough (say, adiabatic, constant-volume) duct, $\epsilon \to 0$, T_ϵ increases, and Θ_ϵ decreases; in such cases, chemical conversion could supplement significantly compression as a mechanism for unburned-gas preheating.

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‡‡Compressional heating exceeds the heat loss to the walls in the end gas for cases of automotive interest. Hence, the end gas is supercritical in the sense that pressure and temperature are assured to rise in time. The concern is whether or not the increase of temperature and pressure in time (from the compressional preheating/heat loss balance) is such that transition to explosion is deferred so that completion of flame propagation occurs instead. Thus, while representing heat loss by adjustment of the polytropic constant precludes study of the near-critical state in which chemical exothermicity and heat loss balance, the present formulation is not aimed at such already well-studied questions.