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Hydrodynamic aspects of end-gas autoignition

Leonid Kagan *, Gregory Sivashinsky

Sackler Faculty of Exact Sciences, School of Mathematical Sciences, Tel Aviv University, Tel Aviv 69978, Israel

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Abstract

Within the small-Mach-number approximation, employing an appropriate scale-separation procedure, a reduced zero-dimensional model for deflagrative combustion occurring in a closed vessel is formulated and analyzed. It is shown that progressive compression of the unburned gas (end-gas) induced by the burned gas thermal expansion may result in end-gas autoignition, provided the vessel is large enough. A theoretical interpretation is given to the effect of the flame velocity reversal occurring prior to the autoignition event.

Keywords: End-gas autoignition; Knocking combustion; Confined burning

1. Introduction

When deflagrative combustion takes place within a confining vessel the unburned gas is progressively compressed owing to thermal expansion of the burned gas. The resulting buildup of the unburned gas (end-gas) reaction-rate may lead, under appropriate conditions, to its autoignition and detonation. The end-gas autoignition is of direct relevance to the familiar knock phenomenon occurring in spark-ignition engines [1,2].

In the one-dimensional geometry (planar, cylindrical or spherical) the closed vessel combustion is one of the most basic and relatively tractable problems of the theory, and there is a substantial volume of literature on the subject [3–10]. The present paper is concerned with some salient features of the problem which somehow escaped proper attention. Specifically, it has long been noticed that the end-gas burning is often accompanied by the reversal of the gas flow, and prior to the autoignition event the flame front is halted and even thrown backward [11–13]. As shown below both effects stem from the end-gas reactivity, and may be successfully tackled theoretically under quite general premises.

The current study is an extension of our recent discussion of the end-gas autoignition based on the small-heat-release approximation, and where the hydrodynamic aspects of the problem stay beyond the scope of the model employed [14].

The small-Mach-number approach discussed below, could presumably be used also to tackle end-charge autoignition in confined solid explosives (Section 8).

2. Small-Mach-number approximation

Since deflagrative combustion is generally strongly subsonic it may be successfully described within the framework of the small-Mach-number approximation. In this limit the end-gas autoig nition (transition to developing detonation) is expected to manifest itself as a drastic amplification

* Corresponding author.
E-mail addresses: kaganleo@post.tau.ac.il (L. Kagan), grishas@post.tau.ac.il (G. Sivashinsky).

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of the end-gas temperature and the mass burning velocity. In this paper the discussion is restricted primarily to the geometrically simplest case of a planar flame confined by two impermeable walls (Fig. 1). For the small-Mach-number limit considered here the pressure is instantaneously equalized throughout the vessel and so is a function of time alone. In suitably chosen units the set of governing equations then reads [7],

heat,

$$\hat{\rho}\left(\frac{\partial \widehat{T}}{\partial \hat{t}}+\hat{u}\frac{\partial \widehat{T}}{\partial \hat{x}}\right)=\varepsilon\frac{\partial^2 \widehat{T}}{\partial \hat{x}^2}+\frac{\gamma-1}{\gamma}\frac{d\widehat{P}}{d\hat{t}}+\frac{1}{\varepsilon}(1-\sigma)\widehat{W} \quad (1)$$

mass fraction,

$$\hat{\rho}\left(\frac{\partial \widehat{C}}{\partial \hat{t}}+\hat{u}\frac{\partial \widehat{C}}{\partial \hat{x}}\right)=\frac{\varepsilon}{Le}\frac{\partial^2 \widehat{C}}{\partial \hat{x}^2}-\frac{1}{\varepsilon}\widehat{W} \quad (2)$$

continuity,

$$\frac{\partial \hat{\rho}}{\partial \hat{t}}+\frac{\partial(\hat{\rho}\hat{u})}{\partial \hat{x}}=0 \quad (3)$$

state,

$$\widehat{P}=\hat{\rho}\widehat{T}, \quad \widehat{P}=\widehat{P}(\hat{t}) \quad (4)$$

reaction rate,

$$\widehat{W}=Z\hat{\rho}\widehat{C}\exp[N(1-\widehat{T}^{-1})] \quad (5)$$

Here $\widehat{P}=P/P_0$ is the scaled pressure in units of the initial pressure, P_0; $\widehat{C}=C/C_0$, scaled mass fraction of the deficient reactant in units of its initial value, C_0; $\widehat{T}=T/T_b$, scaled temperature in units of $T_b=T_0+QC_0/c_p$, adiabatic temperature of burned gas under constant pressure; Q, heat release; T_0, initial temperature; c_p, c_v, specific heats; $\sigma=T_0/T_b$; $\gamma=c_p/c_v$; $\hat{\rho}=\rho/\rho_b$, scaled density in units of the burned gas density $\rho_b=P_0/(c_p-c_v)T_b$; $\hat{u}=u/u_b$, scaled flow velocity in units of u_b, velocity of the open-space (isobaric) deflagration relative to the burned gas, and regarded as a prescribed parameter; $N=T_a/T_b$, scaled activation temperature (energy); Le, Lewis number; $Z=\frac{1}{2}Le^{-1}N^2(1-\sigma)^2$, normalizing factor to ensure that at $N\gg 1$ the scaled deflagration velocity relative to the burned gas is close to unity; $\hat{x}=x/L$, $\hat{t}=u_bt/L$, scaled spatio-temporal coordinates; L, width of the vessel; $\varepsilon=l_{th}/L$; $l_{th}=D_{th,b}/u_b$, flame width; $D_{th,b}=D_{th}(T_b)$, thermal diffusivity of the mixture; $\widehat{W}=(D_{th,b}/C_0\rho_bu_b^2)W$, scaled reaction rate. The reaction rate (W) is assumed to be one-step, irreversible, first-order, and with the Arrhenius temperature dependence.

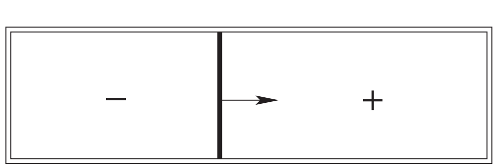

Fig. 1. Diagram for the 1D deflagrative combustion in a closed vessel, $0<x<L$. Bold line corresponds to the reaction zone located at $x=R(t)$; (+) and (−) mark the unburned and burned gas, respectively.

Equations (1)–(4) are considered over the interval $0<\hat{x}<1$ (interior of the vessel), and subjected to the following set of conditions:

boundary conditions,

$$\partial\widehat{T}(0,\hat{t})/\partial\hat{x}=0, \quad \partial\widehat{C}(0,\hat{t})/\partial\hat{x}=0, \quad \hat{u}(0,\hat{t})=0 \quad (6)$$

$$\partial\widehat{T}(1,\hat{t})/\partial\hat{x}=0, \quad \partial\widehat{C}(1,\hat{t})/\partial\hat{x}=0, \quad \hat{u}(1,\hat{t})=0 \quad (7)$$

initial conditions,

$$\widehat{T}(\hat{x},0)=\sigma+(1-\sigma)\exp(-\hat{x}/l), \quad \widehat{C}(\hat{x},0)=1, \quad (8)$$

$$\widehat{P}(\hat{x},0)=1, \quad \hat{\rho}(\hat{x},0)=1/\widehat{T}(\hat{x},0), \quad \hat{u}(\hat{x},0)=0$$

Here l is the length-scale of the initiation hot-spot.

3. Thin flame limit

The model (1)–(5) involves two natural small parameters ε and N^{-1}, which allow for some further simplifications.

In deflagrative combustion the width of the reactive-diffusive zone, by definition, is of the order of ε. Let $\hat{x}=\widehat{R}(\hat{t})$ be a site of the deflagration front (reaction zone). Then beyond the reactive-diffusive layer $\hat{x}-\widehat{R}(\hat{t})\sim\varepsilon$ (outer picture) the profiles of $\widehat{T}$, $\widehat{C}$, $\hat{u}$, $\hat{\rho}$ are expected to be discontinuous:

$$\widehat{T}=\widehat{T}_-(\hat{x},\hat{t}), \quad \widehat{T}_+(\hat{t}); \quad \widehat{C}=\widehat{C}_-(=0), \quad \widehat{C}_+(\hat{t});$$
$$\hat{u}=\hat{u}_-(\hat{x},\hat{t}), \quad \hat{u}_+(\hat{x},\hat{t}); \quad \hat{\rho}=\hat{\rho}_-(\hat{x},\hat{t}), \quad \hat{\rho}_+(\hat{t}) \quad (9)$$

The subscripts −, + mark the burned and unburned gas, respectively. In view of the initial conditions (8), elements of the gas that have not crossed the reaction zone are thermodynamically identical, that is $\widehat{T}_+$, $\widehat{C}_+$, $\hat{\rho}_+$ are $\hat{x}$-independent [7].

For the burned gas interval ($0<\hat{x}<\widehat{R}$) where $\widehat{C}=0$, one may write,

$$\hat{\rho}_-\left(\frac{\partial \widehat{T}_-}{\partial \hat{t}}+\hat{u}_-\frac{\partial \widehat{T}_-}{\partial \hat{x}}\right)=\frac{\gamma-1}{\gamma}\frac{d\widehat{P}}{d\hat{t}} \quad (10)$$

$$\frac{\partial \hat{\rho}_-}{\partial \hat{t}}+\frac{\partial(\hat{\rho}_-\hat{u}_-)}{\partial \hat{x}}=0 \quad (11)$$

$$\widehat{P}=\hat{\rho}_-\widehat{T}_-, \quad \widehat{P}=\widehat{P}(\hat{t}) \quad (12)$$

Similarly, for the reactive gas interval ($\widehat{R}<\hat{x}<1$), where $\partial\widehat{C}_+/\partial\hat{x}=\partial\widehat{T}_+/\partial\hat{x}=\partial\hat{\rho}_+/\partial\hat{x}=0$,