

KINEMATIC MODEL APPLIED TO FLAME PROPAGATION IN CLOSED TUBE WITH VARIABLE VOLUME

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Abstract. In this work the evolution of a premixed flame under confinement and variable volume conditions is studied theoretically. The analysis is based on a hydrodynamic model in which the flame is treated as a surface of discontinuity. Its solution in the post-ignition period yields a coupled system of equations for the determination of the pressure and the burning rate. The burning rate is modeled using empirical correlations. The analysis also solves the thermal and flow fields on either sides of the flame and determines the instantaneous location of the flame front together with the overall time required for the flame to reach the end of the tube. The results indicate that distinct behaviors are possible for different relations of the frequency (ω) and amplitude (A) specified for the variation of the volume of the chamber, with respect to the combustion time and evolution of pressure.

Keywords. Flame propagation, Combustion, Closed Vessel

1. Introduction

Studies of laminar premixed flame propagation in confined vessels have a long history in both experimental and theoretical works. The practical importance of these studies is related to the understanding of processes inside internal combustion engines. Thermodynamic models such as those developed by Bradley and Mitcheson (1976) or Takeno (1979) usually need input from experimental data. Later Sivashinsky (1979) developed a hydrodynamic model for flame propagation in a sphere. In 1992 McGreevy and Matalon constructed a hydrodynamic model that adds the flame structure implemented by Peters and Ludford (1983) which was studied by Sivashinsky (1976), and Matalon and Matkowsky (1982). They substituted it into Sivashinsky's model to describe the propagation of a planar flame in a closed tube. The coupled effect of pressure variation and Lewis number is the main subject of this study. In this case the flame did not experience flame stretch. Tien (1996) developed a model to analyse the propagation of a planar premixed flame in a closed tube of length L with varying cross-sectional area. Effects of flame stretch on flame propagation in a closed tube were investigated.

The recent increase in computational power has permitted the modeling of different aspects of combustion processes with great detail. Comes to all attention to the detailed chemistry calculations, direct numerical simulations of flame turbulence interactions and interactions of flames with boundaries or boundary layers. But the combination of all these detailed models to solve the problem of turbulent flame propagation in complex geometries with detailed chemistry is still a need for simplified computational models that describe only the essential features of the processes involved. Therefore, it is important to thoroughly examine the individual process involved in the flame propagation phenomenon. In this work, the evolution of a premixed flame under conditions of confinement and variable volume is studied theoretically. The analysis is based on a hydrodynamic model in which the flame is treated as a surface of discontinuity. Its resolution in the post-ignition period yields a coupled system of equations for the determination of the pressure and the burning rate. The burning rate is modeled using empirical correlations. The analysis also resolves the thermal and flow fields on both sides of the flame and determines the instantaneous location of the flame front together with the overall time required for the flame to reach the end of the tube. The results indicate that qualitatively distinct behaviors that are possible for different relations of the frequency (ω) and amplitude (A) specified for the variation of volume of the chamber, with respect to the combustion time and evolution of pressure.

2. Model

The model of the flame propagation consists of a homogeneous premixed combustible mixture that occupies a closed tube of length L , Fig. (1). Considering that the curvature of the surface of the flame front is always small in comparison with the thickness of the front, that is, the reaction zone, one may consider, with sufficient accuracy, that all magnitudes of the conserved variables within this zone are functions of a single coordinate, the direction which is perpendicular to the element of front area. In this context, the cross section of the tube is taken to be sufficiently narrow so that variations in the state of the gas occur primarily along the axial direction.

The problem consists in determining the influence of burning rate and variation of volume on the pressure in the vessel after the mixture is ignited at the left end of the tube. Note that the process of combustion occurs under confined conditions and the volume of the chamber undergoes temporal variations. The planar flame is assumed to be established from the beginning. After the mixture is ignited at the left end, a flame propagates throughout the tube, leaving hot burned behind it. It is assumed that combustion occurs under adiabatic conditions.

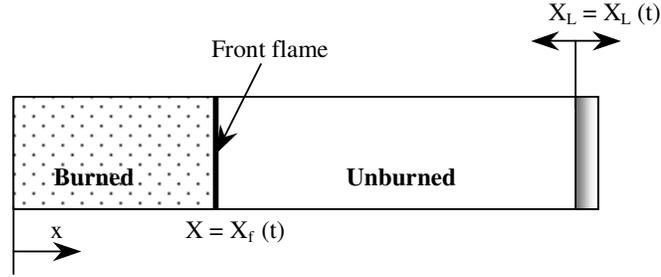


Figure 1. Sketch of flame propagation in a closed tube with variable volume.

3. Governing Equations

The fundamental equations are based on a physical-chemical model that, despite of its simplicity, captures all the most significant features of the hydrodynamics of flame propagation in a confined volume. It is assumed that the propagation of the flame depends on diffusion of a single component A of the mixture, the component limiting the chemical combustion reaction. The combustible mixture is assumed to be a homogeneous perfect gas A_0 . Thus, the thermal conductivity of the mixture depends entirely on the properties of the gas A_0 , while the diffusivity of the component A depends on the binary diffusivity of A in A_0 . To simplify the calculations, it is further considered that the specific heats and transport coefficients are constant, temperature independent parameters. For a detailed description and discussion about this model, refer to the well-known article of Sivashinsky (1977).

Since the propagation velocity of the flame is typically much smaller than the characteristic speed of sound, the representative Mach number is small. As a consequence, the pressure at any instant is practically equalized throughout the tube. The non-dimensional governing equations expressing the balance of mass, momentum, energy, and reactant concentration, supplemented by the equation of state, are:

$$\frac{\partial p}{\partial t} + \frac{\partial \rho u}{\partial x} = 0, \quad (1)$$

$$\rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} = -\frac{\partial p}{\partial x} + \frac{4}{3} \text{Re}^{-1} \frac{\partial^2 u}{\partial x^2}, \quad (2)$$

$$\rho \frac{\partial T}{\partial t} + \rho u \frac{\partial T}{\partial x} = \delta \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) + \delta^{-1} q D (\rho Y)^n e^{-\frac{\theta}{T}} + \frac{\gamma-1}{\gamma} \dot{P} - (\gamma-1) \frac{P}{V} \frac{dV}{dt}, \quad (3)$$

$$\rho \frac{\partial Y}{\partial t} + \rho u \frac{\partial Y}{\partial x} = \frac{\delta}{\text{Le}} \frac{\partial}{\partial x} \left(\lambda \frac{\partial Y}{\partial x} \right) - \delta^{-1} D (\rho Y)^n e^{-\frac{\theta}{T}}, \quad (4)$$

$$\rho T = P. \quad (5)$$

In this formulation, $u = u(x,t)$ is the axial velocity component, $T = T(x,t)$ temperature, $P = P(t)$ pressure and $Y = Y(x,t)$ reactant mass fraction. The coordinate x is the distance along the tube. The variable $V = V(t)$ is the volume of the chamber. An irreversible one-step chemical reaction has been

assumed, with an overall reaction of order n . The dimensionless parameters appearing in the governing equations are the heat release q , Reynolds number Re , Lewis number Le and activation energy θ . By definition:

$$q = \frac{Q Y_0}{c_p T_0}, \quad (6)$$

$$Re = \frac{M_0 L}{\mu}, \quad (7)$$

$$Le = \frac{\lambda}{\rho D c_p}, \quad (8)$$

$$\theta = \frac{E}{RT_0}. \quad (9)$$

Should be noted that the temperature dependence of the reaction rate is of Arrhenius type with an activation energy E . The state of the fresh mixture is taken as the reference state using the parameters ρ_0 , p_0 and T_0 . The burning rate of an unconfined adiabatic plane flame M_0 is chosen as a unit of mass flux. The parameters μ and λ represent the viscosity and thermal conductivity. The Damköler number D is chosen as to ensure that the dimensionless burning rate of an unconfined flame, in the limit $\theta \rightarrow \infty$, is unity. Lengths are nondimensionalized with respect to L and time, t , with respect to $\rho_0 L / M_0$. The problem involves an additional length scale associated with diffusion, namely:

$$L_D = \frac{\lambda_0}{c_p M_0}, \quad (10)$$

The ratio $\delta = L_D / L$, therefore, characterizes the flame thickness. In the limit $\delta \rightarrow 0$, the flow field consists of two distinct fluid-dynamic zones, where diffusion and chemical reaction are negligible, separated by the flame front. Restricting the model to leading order and introducing the transformation $z = \int_0^x \rho(x', t) dx'$, equations (1), (3) and (4) become:

$$\frac{\partial u}{\partial z} = -\frac{1}{\rho^2} \frac{Dp}{Dt}, \quad (11)$$

$$\rho \frac{DT}{Dt} = \frac{\gamma-1}{\gamma} \dot{P} - (\gamma-1) \frac{P}{V} \dot{V}, \quad (12)$$

$$\frac{DY}{Dt} = 0, \quad (13)$$

where $\frac{D(\cdot)}{Dt}$ is the lagrangean operator. These equations are to be satisfied on either side of $z = Z_f$.

3.1. Jump Relations

The methodology adopted in this work is similar to the one used by McGreevy and Matalon (1992). A substitution of the equation of state, Eq. (5), into the energy equation, Eq. (12) leads to:

$$\frac{D}{Dt} \left(\frac{P}{\rho} \right) = \frac{(\gamma-1) \dot{P}}{\gamma} - (\gamma-1) \frac{P}{\rho} \frac{\dot{V}}{V},$$

which, after some algebraic manipulations, becomes:

$$\frac{D\varepsilon}{Dt} = 0, \quad (14)$$

where $\varepsilon = \frac{P^{\frac{1}{\gamma}}}{\rho V^{\gamma-1}}$ is an entropy function. Equation (14) means that on each side of the flame the entropy of individual fluid elements is conserved. Since the entropy in the fresh mixture is initially uniform,

$$\varepsilon = \begin{cases} 1 & z_f < z < 1, \end{cases} \quad (15a)$$

for all times. The flow in the burned gas region, however, is rotational. A curved flame generates vorticity because the flow is bent (toward the normal direction) on passing through the flame front. Hence, the flow field must be determined by solving the coupled equations developed for mass, momentum and energy. Considering a planar flame, while accounting for Eq. (14), yields:

$$\varepsilon = \begin{cases} \varphi(z) & 0 < z < z_f. \end{cases} \quad (15b)$$

Similarly, Eq. (13) states that the reactant concentration of individual fluid elements is conserved. From the equations (11), (12) and (13), the solutions for T, Y and ρ to leading order are:

$$T = \begin{cases} P^{\frac{\gamma-1}{\gamma}} V^{\gamma-1} \varphi(z) & 0 < z < z_f, \\ P^{\frac{\gamma-1}{\gamma}} V^{\gamma-1} & z_f < z < 1, \end{cases} \quad (16)$$

$$\rho = \begin{cases} \frac{P^{\frac{1}{\gamma}}}{V^{\gamma-1} \varphi(z)} & 0 < z < z_f, \\ \frac{P^{\frac{1}{\gamma}}}{V^{\gamma-1}} & z_f < z < 1 \end{cases}, \quad (17)$$

$$Y = \begin{cases} 0 & 0 < z < z_f, \\ 1 & z_f < z < 1. \end{cases} \quad (18)$$

The continuity equation, Eq. (11), can now be integrated to give:

$$u = \begin{cases} \left[(\gamma-1) \left(\frac{V^{(\gamma-1)}}{P^{\frac{1}{\gamma}}} \right) \frac{\dot{V}}{V} - \frac{1}{\gamma} \left(\frac{V^{(\gamma-1)}}{P^{\frac{1}{\gamma}}} \right) \frac{\dot{P}}{P} \right] \int_0^{z_f} \varphi(z) dz & 0 < z < z_f, \\ \left[u_{\text{pistão}} - (\gamma-1) \left(\frac{V^{(\gamma-1)}}{P^{\frac{1}{\gamma}}} \right) \frac{\dot{V}}{V} - \frac{1}{\gamma} \left(\frac{V^{(\gamma-1)}}{P^{\frac{1}{\gamma}}} \right) \frac{\dot{P}}{P} \right] (1-z) & z_f < z < 1 \end{cases}. \quad (19)$$

Insight into the flow characteristics in these conditions may be obtained from Eq. (19). Considering the volume of the chamber is constant, Eq. (19) comes down to Eq. (21) of McGreevy and Matalon (1992). The fresh unburned gas is compressed and pushed toward the right end of the tube, while the burned products move away from the flame toward the left end of the tube. However, depending on the rate of variation of the volume, this behavior can change because the gas speed clearly depends on the rate of pressure buildup and the volume.

3.2. Evolution of Pressure and Burning Rate

Integrating Eq. (3) across the flame yields, to leading order in δ ,

$$T(z = z_f^-) - T(z = z_f^+) = q, \quad (20)$$

from which the relations (21) and (22) follow:

$$T(z = z_f^-) = q + P^{\frac{\gamma-1}{\gamma}} V^{\gamma-1} \quad \text{and} \quad (21)$$

$$\varphi(z_f) = 1 + q P^{\frac{1-\gamma}{\gamma}} V^{\gamma-1}. \quad (22)$$

By definition, the burning rate is calculated as a function of the rate of burned gas produced by combustion, namely:

$$M = \dot{z}_f = \frac{d(\rho_{\text{burned}} V_{\text{burned}})}{dt} . \quad (23)$$

Combining the Eqs. (16), (17), (22) and (3), it is obtained:

$$\frac{d(PV)}{dt} = \gamma q M . \quad (24)$$

Note that once Z_f is known, Eq. (22) provides an implicit way of determining the functional relationship $\varphi(z)$. It remains, however, to determine the burning rate M for which the details within the flame zone are essential. The phenomena involved in slow flame propagation lead to the property of the flame front; namely, of a definite quantity z grams of mixture burned per unit area of surface or, alternatively, of being propagated relative to the non-burning gas in a direction normal to its surface with a propagation velocity S_f centimeters per second. The observed motion of the flame is the result of the superposition of all kinds of hydrodynamic motions upon the fundamental motion of the flame front. By definition:

$$M = \dot{z}_f = \rho_{\text{burned}} S_f A_f , \quad (25)$$

where A_f is the front flame area. Similarly to Karlin *et al.* (2000), this work uses an empirical correlation to calculate S_f . The relation (26), shown below as an example, is due to Metagalque (1987-ver).

$$S_f = \psi \frac{T_{\text{unburned}}^\alpha}{P^\beta} . \quad (26)$$

The parameter ψ and the coefficients α and β are obtained experimentally. Using Eqs.(17) and (25), it is obtained:

$$\frac{dz_f}{dt} = \psi \frac{P^{(\alpha-\beta)(1-\alpha)/\gamma}}{\varphi(z_f)} A_f . \quad (27)$$

The system composed of Eqs. (24) and (27) consists of the a closed system of differential equations representing the confined combustion in the interior of a tube with variable volume. This system can be integrated numerically using, for instance, the Runge Kutta method.

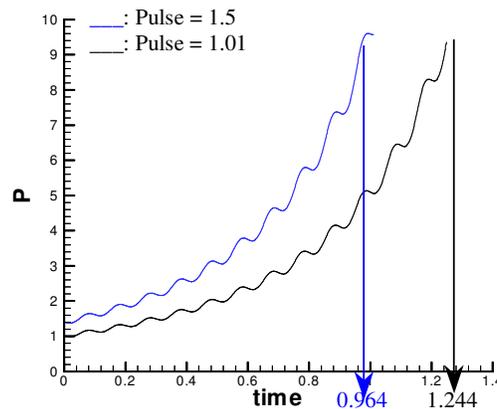
4. Results

The results are presented in terms of the parameters shown in Tab. (1). Typically values of ψ , θ and the coefficients α and β were defined for that $q \approx 6$. The geometry of the first case study is shown in Fig. (1). The function X_L is defined as $X_L = 1 + A \cdot \text{SIN}(\omega t)$. The functional dependence of the pressure with the time is shown in Fig. (2a). Two aspects can be observed: the exponential increasing of the oscillations of pressure even through the volume change has been maintained under a constant rate. This fact clearly shows the influence of the excitation of frequency in the burning process. With respect to the largest pressure in the system, it does not occur at the final burn time. Essentially, it depends on the coincidence of phase between pressure and volume of the chamber. The variation of the burning rate with the product of pressure and volume (PV) is shown in Fig. (2b). The results indicate that, after a short initial adjustment, the burning rate M becomes independent of the initial condition and increases continuously with PV. However, there is a considerable influence of the initial conditions on the evolution of pressure in the chamber, typical of oscillatory processes. Finally, the dependence of Z_f on PV is presented in Fig. (2c). It can be verified that the form $Z_f = B.(PV)^a$ is a reasonable approximation and independent of initial conditions. Therefore, the correct determination of the coefficients 'a' and 'B' is a very important step in combustion system projects.

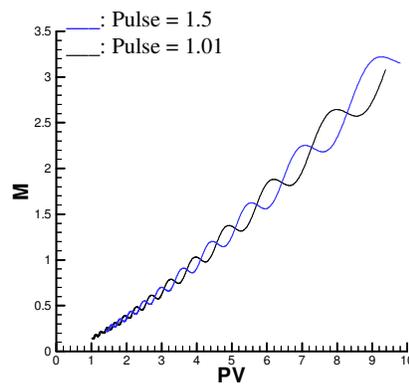
The dependence of the burning time and pressure with the amplitude and frequency is depicted in Fig. (3). The signal of the amplitude indicates the initial direction of the movement of the piston. The absolute value of the amplitude indicates the maximum amplitude allowed. The time required for the flame to reach the right end of the tube is obtained as the time when $Z_f = 1$, that is to say, when all mass of gas has been burned. An interesting observation is that there is a range of the frequencies in which it does not occur any burning time change. This may be attributed to the fact that the rate of compression of the mixture does not influence significantly the burning rate anymore. According to Fig. (3), one can distinguish two cut frequencies in the range of the present simulations. Additional field details may be observed from the analysis of the burning time. The high negative amplitudes lower the burning time. This behavior can be ascribed to the low volumes and, in consequence, high density. Since the burning rate is directly proportional to the burned gas density, the burning time will be lower in this range of analysis. Finally, should be noted that the product between the final pressure and volume of the vessel is always constant for all cases analyzed in this work. Figure (3) consists of an envelope for the use in the optimization of combustion processes.

Table 1. Standard simulation.

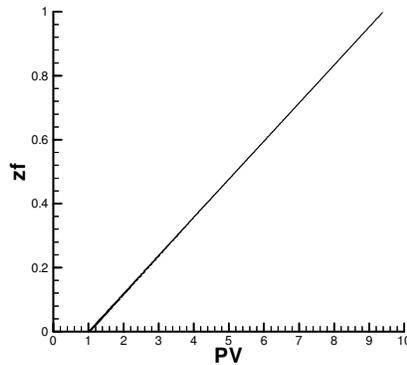
Parameter	Non-dimensional Value
α	2.3
β	0.23
ψ	1.
γ	1.4



(a) Variation of pressure with respect to time ($f = 10$, $A = -0.05$);



(b) Variation of burning rate with respect to pressure ($f = 10$, $A = -0.05$);



(c) Variation of burning mass with respect to the product of the pressure and volume
 ($f = 10$, $A = -0.05$, Pulse = 0.01) ;

Figure 2. Dependence of burning rate (M) on pressure (P) – case of periodic variable of volume. $x_L = 1 + A \cdot \text{SIN}(\omega t)$.

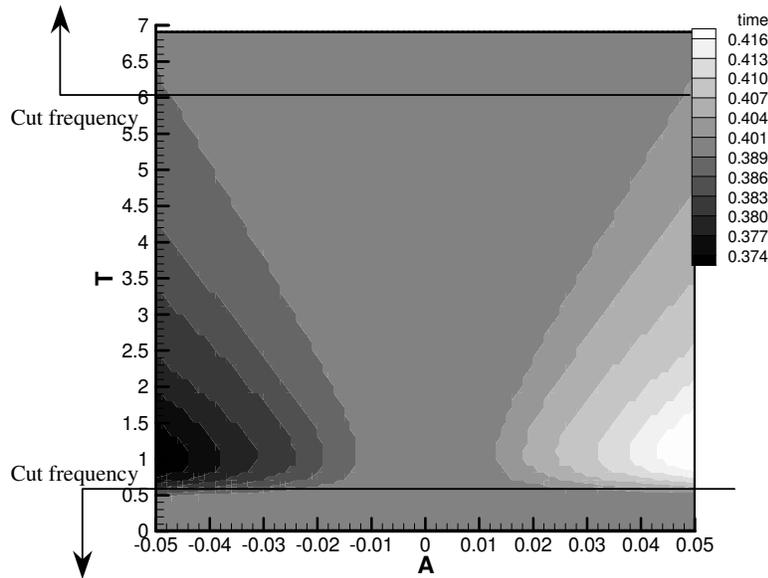


Figure 3. Frequency field indicating the dependence of burning time on frequency ($1/T$) and amplitude (A) – Pulse = 1.01, $\psi = 3$. – case of periodic variable of volume. $x_L = 1 + A \cdot \text{SIN}(\omega t)$.

The geometry of the second case study is illustrated in Fig. (4). The results are presented in terms of the parameters shown in Tab. (2). V_{init} is the initial velocity of the piston. The negative sign indicates the initial direction of the piston. $X_{L,init}$ designates the initial position of piston. In this case, the function X_L is computed with both the pressure and burning rate. The governing equation of this movement obeys the Newton law (Rao, 1985). The variable k , which determines the fundamental frequency of the device of variable volume, has been defined as the stiffness of the spring. In fact, this simulation differs from first case since there is an interaction between the moving flame, in consequence the thermo-fluid dynamics of the gas in the chamber, and piston. This dependence is depicted in Fig. (5). According to Fig. (5a) lower stiffness values decrease the burning time. This fact can be assessed using the Fig. (5b) and (5c). Should be noted that a high reduction in volume causes a high burning rate. In this case, it prevailed the higher reduction volume rate, due to initial velocity of the piston, than the oscillations, characteristics of the stiffness of the spring, under the burning time. However, in systems that present higher frequency, the oscillation effect is more important than the initial velocity of the piston.

Again, it is observed that there is a range of the frequency for which it does not occur any burning time change. For stiffness $k < 0.01$, practically, burning time changes are negligible. The burning rate behavior is shown in Fig. (5c). Analogously, for stiffness $k > 100$, the burning behavior is similar to burning with constant volume.

Table 2. Standard simulation – case of variable of volume by equation of motion for forced vibration

Parameter	Non-dimensional Value
k	Indicate in figure
Pulse	1.01
V_{init}	-1.
X_{Linit}	1.
ψ	1.

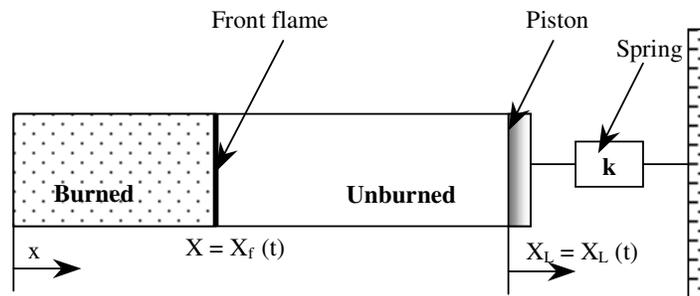
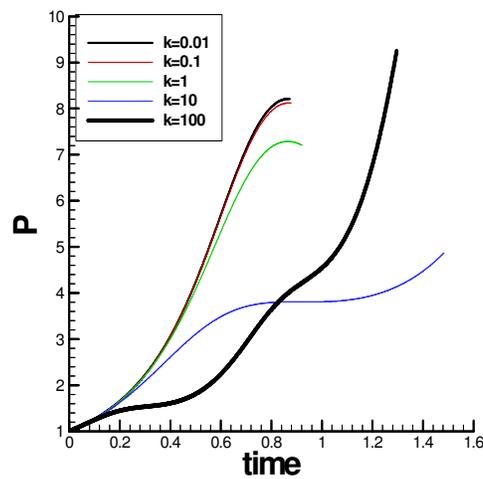
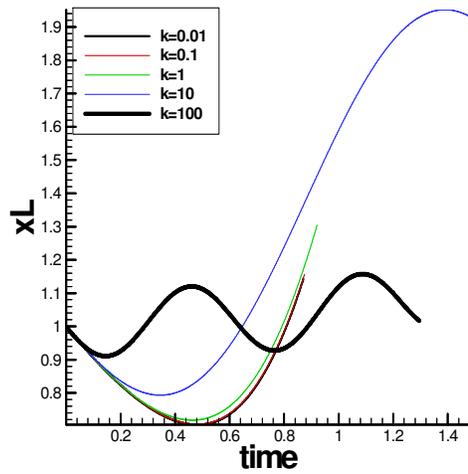


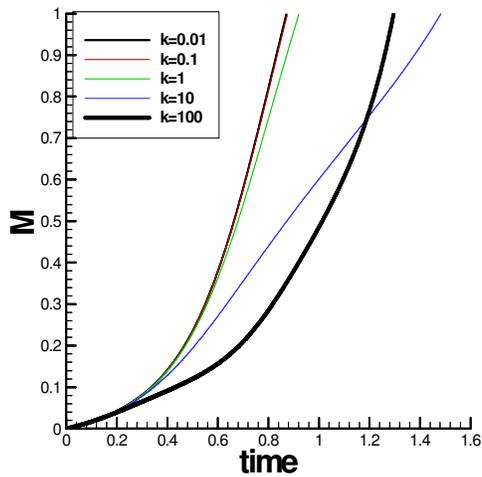
Figure 4. Sketch of flame propagation in a closed tube with variable volume by forced vibration.



(a) Variations in pressure as a function of time;



(b) Variations in position of the piston with respect to time;



(c) Variations in burning rate with the time;

Figure 5. Curves indicating the dependence of the burning rate and pressure with time – case of variable of volume by equation of motion for forced vibration;

Finally, the variations of the unburned gas velocity and the flame velocity as functions of the volume of the chamber are shown in Fig. (6), for two different values of spring stiffness. According to Eq. (19), the unburned gas velocity can assume negative values. An important difference between the burning processes at constant volume and variable volume is the signal of unburned gas velocity. Flexible systems lead to greater negative velocities due to greater reduction in the volume and, consequently, to greater burning rates.

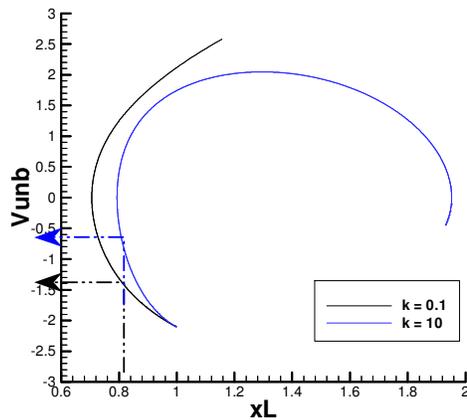


Figure 6. Behavior of the unburned gas velocity with respect to time – case of variable of volume by equation of motion for forced vibration;

5. Conclusions

The evolution of a premixed flame under conditions of confinement is studied theoretically. This work is restricted to flames propagating in narrow channels with thermally insulated walls. Furthermore, the assessment of the burning rate is particularized for cases showing functional dependence with respect to pressure and temperature. The coefficients characterizing this functional dependence are determined experimentally. The results indicate that distinct behaviors are possible for different values of frequency and amplitude of excitation. The present method is a viable alternative for estimation of the pressure and burning rate in systems for which the volume change and the burning rate functions are known. The practical importance of these studies is related to the understanding of processes inside internal combustion engines and burning processes. In addition, the computational cost of this method is negligible compared to a similar study using the Computational Fluid Dynamics (CFD) technique. This fact makes this method suitable for validation of CFD codes.

6. References

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