

The role of compression waves in flame acceleration and transition to detonation inside confined volumes

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Abstract. Features of the unsteady flames propagating in channels filled with gaseous combustible mixtures are studied numerically. The analysis is based on the model treating the flame as a moving energy source. It is shown that the crucial role in flame dynamics and its structure evolution belongs to the compression waves emitted by non-steady flame itself. The compression waves establish flow pattern, temperature and pressure fields near the flame front, which in turn determine the features of flame evolution on the different stages of its propagation.

1. Introduction

For decades, clear understanding of the non-steady and transient regimes of gaseous combustion remained to be a topical problem of the combustion theory, as it was important for the explosion safety and propulsion systems design. However, in spite of wide range of experimental data there is still no systematic analysis of the studied phenomena. The aim of the paper was to resolve the features of the unsteady flames propagating through gaseous combustible mixtures at different external conditions intrinsic to the real technical system environment. It is well known that the flame propagating through the channel evolves in a close feedback with the flow. The feedback occurs in following stages: non-steady (accelerating) flame emits compression waves, this compression waves transfer momentum to the flow, determining the flow pattern near the flame front. In turn, the flow evolution causes flame surface stretching that defines further flame acceleration or deceleration. Usually to describe this process in specific conditions one assumes the flame to be a gasdynamical discontinuity acting as a piston (or semi-transparent piston) compressing the gaseous media. Here we decided to analyze the feature of flame evolution and its compression effect on the flow inside the channel treating the flame as an energy release zone of the finite width. Such a flame structure can be reproduced numerically with a good accuracy using the reduced chemical kinetics and standard transport models (see e.g. [1]).

First, it is useful to emphasize the basic features of flame dynamics and possible combustion regimes within semi-closed channels. Frequently the flames propagating through the channels were of interest in view of studying the flame acceleration and transition to detonation phenomena (see e.g. [2–4] etc.). In highly reactive oxy-fuel mixtures (of hydrogen, acetylene, ethylene etc.) the detonation can be obtained in smooth channels of relatively small width [3–6]. Flame evolution in smooth channels can be described in following basic stages. On the early stage, the flame ignited near the endwall propagates mainly due to the expansion of the hot combustion products out from the ignition zone. The flame propagating with initially normal



laminar speed accelerates in exponential-like regime determined by the linear feedback between the laminar flame and the flow. After some period, the flame dynamics transits in non-linear stage. On this stage, the flame can even decelerate or propagate in oscillatory regime. Finally, the flame can reach the sonic speed and its further acceleration may trigger the onset of detonation. The characteristic flame speed evolution is shown in figure 1 ($U_{f,L}$) for the case similar to described in [3,4].

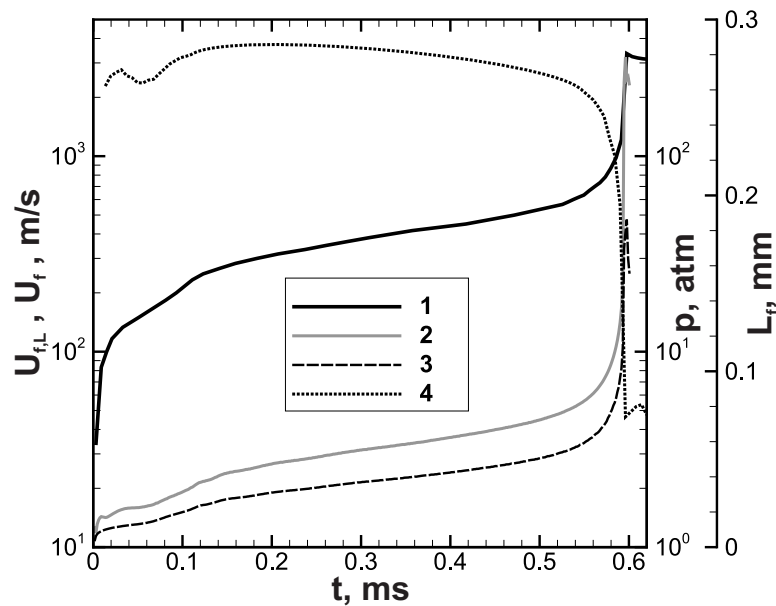


Figure 1. Time evolution of flame characteristics propagating through the semi-opened channel filled with stoichiometric hydrogen-oxygen mixture at initial normal conditions.

2. Problem setup

The results presented below are obtained numerically for initially planar flame propagating through the semi-closed smooth channel filled with hydrogen-oxygen stoichiometric mixture using the mathematical models, program codes and problem setup described in our previous papers (see [7,8]). As it was shown recently in [8] the pattern of the process evolving in two-dimensional channel is qualitatively similar to the real three-dimensional one. Therefore, here we present results of two-dimensional solution for the flame propagation in abovementioned conditions. To resolve chemical kinetics we used reduced kinetic scheme by Warnatz. The system of two-dimensional gasdynamics equations was solved using the euler-lagrange algorithm [9] modified and approved in our previous papers (see [7,8] and references within). The stiff system of reaction kinetics differential equations were solved using the Gear method from the standard mathematical library SLATEC. According to our recent experience, the chosen approach based on the mentioned numerical methods for gasdynamics and reaction kinetics provides a high accuracy while studying numerically the transient regimes of ignition, combustion and detonation. Fine enough computational meshes were resolved with use of computational facilities of the Joint Supercomputer Center of the Russian Academy of Sciences.

3. Results and discussion

To understand the features of the compression waves and flows induced by an accelerating flame first let consider a freely propagating flame. Such an unconfined flame can be observed

in the open spaces [10] or on the first stage after ignition inside the closed chamber near the ignition zone. Unconfined flame can be treated as an energy release zone of a given width (flame width) propagating with a given speed (flame speed). Such a moving energy source irradiates compression waves in every direction. In case of unconfined diverging flame, the waves propagating upward to the center of the flame first converge with amplification and then after passing the center diverge with attenuation. On the early stage when the flame radius is relatively small these waves may outrun the flame front as they propagate with a sonic speed in combustion products (a_b) that is much greater than the combustion speed (U_f). This phenomenon determines the expansion of the combustion products and flame acceleration on this stage up to the visible flame speed $U_{f,L} = \theta U_f$, where θ – is an expansion factor determined as a relation of the densities of cold fuel (ρ_f) and hot combustion products (ρ_b). The compression waves going outward attenuate relatively fast giving insufficient value of momentum to the gas ahead the flame front. Therefore there is no further acceleration of the flame due to the positive feedback between the flame front and the flow ahead.

When studying the flame propagating through the channel out from the closed end one should observe less attenuation of the compression waves going downward (the compression waves in the channel are approximately planar). The waves transfer momentum and energy to the gas ahead the flame front, consequently every further wave propagates through more compressed and heated media with a higher speed. As a result, the flow ahead the flame front accelerates involving the flame in the accelerating movement.

As the flame moves through the channel the role of compression waves, propagating in the opposite direction, changes. Those waves propagate in the direction towards the closed end of the channel with sonic speed in combustion products (a_b), reflect from it and move towards the flame front. On the early stages of flame acceleration as the distance between closed end and the flame front is relatively small ($X_f \sim 0$) and the flame front moves with low velocity $U_{f,L} \ll a_b$ compression waves reflected from the closed end overtake the flame. This phenomenon equalizes the pressure behind the flame front and supplies the flow ahead the flame front with additional amount of momentum and energy. On the other hand asymptotically flame velocity accelerates up to the maximum possible velocity equals to the sonic speed in combustion products $U_{f,L} \sim a_b$ and passes long distance ($X_f \gg 0$) from the end of the channel so compression waves irradiated in upwind direction could not catch up the flame front and affect its dynamics after reflection from the closed end of the channel. The existence of these two asymptotes tells one about the existence of the intermediate flame propagation stage when the influence of compression waves reflected from the closed end of the channel reduces drastically but still remains. Compression waves interact with each other in the combustion products area between flame front and closed end of the channel. They interfere and can generate weak shocks that are able to overtake flame front and affect flame dynamics in a discrete way. On this intermediate stage pressure equalization between flame front and channel closed end takes much longer time than on initial stages of the process. With decreasing the influence of reflected compression waves on the flame front, one can cognize a pressure spike inside the reaction zone that increases during energy source (flame front) propagation. Characteristic pressure profile evolution during flame acceleration process is given on figure 2. Here pressure spike emergence time instance is marked “1”.

Compression waves propagation determines flow acceleration and hence flame acceleration which velocity can be derived as $U_{f,L} = U_f + u_f$ where u_f is the local velocity of the flow. On the early stages, compression waves develop the flow with following velocity profile ahead the flame front: velocity has uniform value in the bulk and decelerates in the boundary layers down to the zero. During this stage, initially planar flame adopts to this flow structure, which determines the stretching of its surface. Flame surface increase gives rise to ΔV —the volume of the fresh mixture consumed by the reaction zone. Therefore the flame velocity increases as

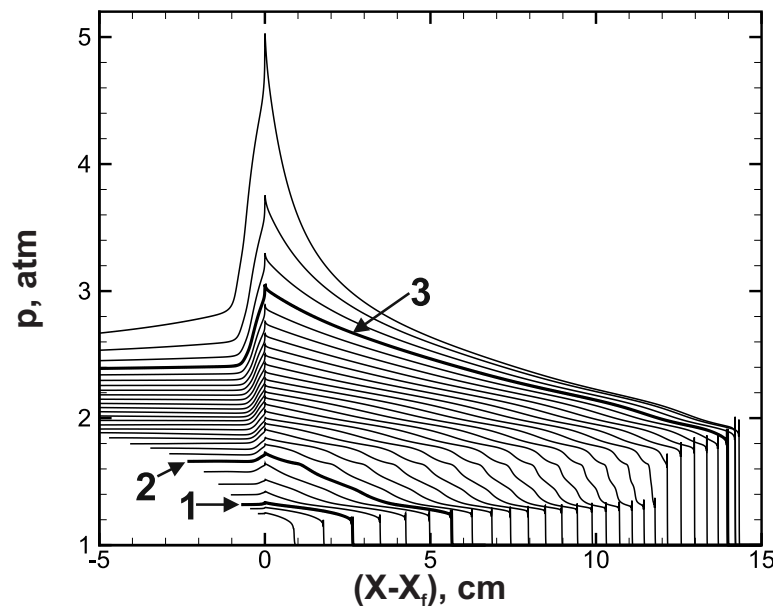


Figure 2. Pressure profile evolution in the coordinate system moving with the flame leading edge ($t_0 = 10 \mu s$, $\Delta t = 20 \mu s$). The specific time instants are marked with numbers: “1”—the pressure peak formation starts, “2”—the initial stage characterized by exponential velocity increase transits into the sub-exponential stage, “3”—the flame achieves sonic speed in the fresh mixture ahead of its front.

$U_{f,L} = \Delta V / S \Delta t$. On the other hand volume of the mixture consumed by the reaction zone per unit time linearly depends on the velocity of the flow ahead the flame $\Delta V \sim u_f$. These relations describe linear feedback between the flow induced by the accelerating compression waves and the accelerating flame that propagates in the channel with exponential velocity increase as in accordance to derived relations $\Delta U_{f,L} \sim \Delta u_f \sim U_{f,L}$ and $U_{f,L} \sim \exp(\alpha t)$. During the process of flame adaptation to the flow the leading role belongs to the compression waves emitted towards side walls of the channel. Their reflection from the sidewalls and interaction with the flame surface determines the stabilization of the flame front surface. It should be noted that on the exponential stage of flame acceleration ($t = \{0.02 - 0.12\} ms$ in figure 1) one can see that flame front thickness (L_f) increases by about 10% against initial value $L_f \sim 0.26 mm$, while burning velocity U_f doubles. That is connected with preliminary compression and heating of the fresh mixture consumed by the flame front. In case of flame propagating via thermal conductivity phenomenon relation between flame front thickness and burning velocity is following $L_f \sim \lambda / U_f$, where λ is effective thermal conductivity. According to this relation, flame-front thickness should decrease with burning velocity rise, reverse result indicate dominating gasdynamical nature of flame development on this stage.

As the flame adapts to the flow structure flame velocity increase is no longer exponential (ending of the exponential stage is marked as “2” in figure 2). Flame transits into the intermediate stage described above. Discrete weak shocks outrun the flame front and transfer additional momentum and energy to the flow that causes flame surface stretching by local acceleration of separate areas of the flame surface. The instability and increase of the flame surface under such a discrete external influence is intrinsic for the flame propagating through the channel and can be achieved from the qualitative pattern obtained in [11]. A discrete character of the shock-influence can cause oscillations of the flame speed.

Independently from the flame acceleration mechanism as flame velocity achieves local sonic speed in fresh mixture directly on the front leading edge ($U_{f,L} = a_f$) the nature of interaction between flame and emitted compression waves drastically changes, and compression waves become to play the main role in further process development. Waves emitted from the leading edge of the flame front appear to be localized by the supersonic flow ahead of the flame's leading edge and no longer propagate in downwind direction. They are lag behind the leading edge of the flame and propagate through the reaction zone towards combustion products, compressing the mixture inside the reaction zone (time instance marked "3" in figure 2). Hence perturbations do not propagate downwards the leading edge of the flame front acts like a solid piston propagating inside the fresh mixture with subsonic speed $U_f = U_{f,L} - u_f$, where u_f is a local mass velocity near the leading edge of the flame front. This causes additional compression of the mixture ahead of the flame front and ensures the supply of more heated and compressed mixture inside the reaction zone. Burning velocity on this stage depends on the features of chemical kinetics under continuously elevating pressure ahead and inside the reaction zone. In present case of hydrogen-oxygen stoichiometric mixture burning velocity increases with pressure causing significant acceleration of the flame on this stage. As flame accelerates up to the sonic speed in the combustion products already rear edge of the flame front moves in a piston manner causing additional compression of the medium inside the reaction zone. Perturbations emitted by the leading edge of the flame front do not pervade through the surface of piston-like rear edge of the flame front. They interact with each other and with compression waves emitted by the rear edge of the flame front on the scales of the flame front causing further pressure increase in the reaction zone while flame front thickness decreases significantly (see figure 1). Interaction between compression waves on the scales of the flame front leads to strong shock wave formation that determines combustion wave transformation into the detonation wave. Compression waves emitted towards combustion products remain localized inside reaction zone. Their interaction causes second shock wave formation that overcomes sonic barrier on rear edge of the flame front and propagates towards combustion products. This wave is also called retonation wave.

4. Conclusions

Suggested approach of treating the flame front as moving energy source that emits compression waves allows one to describe in detail all the stages of transient combustion wave development process during propagation inside the closed volume. In particular in present work based on this model comprehensive analysis of the flame acceleration process in channels filled with hydrogen-oxygen mixture is given. Three main stages of the process are highlighted. On the first stage flame front and the flow ahead of it undergo continuous impact of the compression waves emitted from the reaction zone in all the directions. The continuous manner of interaction defines the positive feedback between the flow and flame acceleration that in turn determines the exponential rate of acceleration. The influence of the transverse compression waves travelling between the sidewalls diminishes as the flame adapts to the flow structure developed in channel. The manner of the influence of the compression waves travelling through the combustion products in the gap between the flame front and the back wall becomes discrete as the flame propagates relatively far from the back wall. The compression waves interact with each other behind the flame front producing stronger compression waves or even weak shocks. The discrete impacts of such waves on the flame front determine the features of the flame evolution during the following sub-exponential stage of flame acceleration. Finally after the flame becomes supersonic the emitted perturbations occur to be choked inside the reaction zone determining further compression of the reaction zone resulting on the one hand into the burning velocity increase and on the other hand into the strong shock formation on the scales of the reaction zone. Thus the transition to detonation takes place.

Acknowledgments

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References

- [1] Warnatz J, Maas U and Dibble R W 2001 *Combustion: Physical and Chemical Fundamentals, Modeling and Simulation, Experiments, Pollutant Formation* (Berlin: Springer-Verlag)
- [2] Bivol G Yu, Golovastov S V, Ivanov K V, Korobov A E and Golub V V 2015 *J. Phys.: Conf. Series* (in press)
- [3] Salamandra G D, Bazhenova T Y and Naboko I M 1959 *Proc. Combust. Inst.* **7** 851
- [4] Kuznetsov M, Alekseev V, Matsukov I and Dorofeev S 2005 *Shock Waves* **14** 205–15
- [5] Utriw P A and Oppenheim A K 1966 *Proc. Roy. Soc. A* **295** 13–28
- [6] Wu M *et al.* 2007 *Proc. Comb. Inst.* **31** 2429
- [7] Ivanov M F, Kiverin A D and Liberman M A 2011 *Phys. Rev. E* **83** 056313
- [8] Ivanov M F, Kiverin A D, Liberman M A and Yakovenko I S 2013 *Int. J. Hydrogen Energy* **38** 16427
- [9] Belotserkovsky O M and Davydov Yu M 1982 *Coarse-Particle Method in Hydrodynamics* (Moscow: Nauka, Mir)
- [10] Gostintsev Yu A, Istratov A G and Shulenin Yu V 1988 *Combustion, Explosion and Shock Waves* **24** 563–9
- [11] Deshaies B and Joulin G 1989 *Combust. Flame* **77** 201