Theory of Flame Acceleration in Tubes due to Wall Friction: Intrinsic Limitations and Accuracy

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A slow, subsonic flame can accelerate spontaneously, with the velocity jump by several orders of magnitude and even subsequent detonation triggering. This effect is extremely crucial, in particular, for fire safety issues in mines, subways and power plants. Flame acceleration is especially strong while propagating in tubes or channels. According to the celebrative Shelkin model, the key element of the process is wall friction at non-slip walls. Indeed, as a flame front propagates from a closed tube/channel end to the open one, the burning matter expands and it drives a flow of the fresh fuel mixture. However, due to the friction on the tube walls, the flow becomes non-uniform such that the burning matter bends the flame front, increases the flame velocity and leads to the flame acceleration. During the recent years, the effect has been clarified and investigated – analytically, computationally and experimentally. In particular, the analysis of Bychkov et al. describes the entire scenario of the flame acceleration and detonation triggering, namely: (i) initial exponential acceleration in the quasi-incompressible state; (ii) moderation of the process because of gas compression, so the exponential acceleration state goes over to a slower one; (iii) eventual saturation to a steady, quasi-steady or statistically-steady, high-speed flames correlated with the Chapman-Jouguet deflagration; at the latter stage, heating of the fuel mixture leads to an explosion ahead of the flame front, which develops into a self-sustained detonation. While this analytical theory is validated by extensive direct numerical simulations of the combustion equations including transport process, chemical reactions, viscosity, thermal conduction and diffusion, it nevertheless includes a set of assumptions such as the large Reynolds number related to flame propagation, $Re>>1$, as well as the large thermal expansion coefficient in the burning process, $\Theta>>1$. This therefore leads to the intrinsic limitations of the theory. In this work we determine these limitations and thereby clearly underline the validity domains in the relevant $Re-\Theta$ diagram. The present analysis also demonstrates that the theory of flame acceleration is consistence with a model of steady flame propagation developed recently.

1. Introduction

Two regimes of premixed burning are well-known, namely, a slow subsonic regime of flame (deflagration) and a fast supersonic regime of detonation. For the same fuel mixture, the velocities of a flame and a detonation typically vary by three-four orders of magnitude. However, a flame in a tube or channel can spontaneously accelerate until it triggers a detonation (Shelkin, 1940; Williams, 1985; Zeldovich et al., 1985; Shepherd et al., 1992; Kerampran et al., 2000; Roy et
which states one of the most important and, also, one of the complicated problems in combustion science.

Various experimental studies have shown the following steps in the transition: a flame accelerates, pushes compression waves and weak shocks, which interact, get stronger, compress and heat the fresh fuel mixture, which finally explodes somewhere between the leading shock and the flame front and evolves into the detonation. However, until recently there was very limited theoretical understanding of the flame acceleration, stating the reason and the most important part in the deflagration-to-detonation transition (DDT) event. The first explanation of the acceleration was suggested by Shelkin in the classical work (Shelkin, 1940), see also (Zeldovich et al., 1985); it is related to the non-slip boundary conditions at the walls. As a flame front propagates from a closed tube end, the burning matter expands; it pushes a flow of the fresh fuel mixture; friction at the tube walls makes the flow non-uniform, which bends the flame front, increases the flame velocity and thereby the flame accelerates. Based on this idea Shelkin has proposed a semi-empirical criterion of flame acceleration, according to which any realistic flame with large density drop at the front is expected to accelerate from a closed tube end. However, since the time of Shelkin, there was a common opinion that flame acceleration is impossible without external turbulent flow. That was a fatal trouble for constructing the acceleration theory, because turbulent burning is a key problem of combustion science, which has not been solved yet despite of almost a century of intensive research, see, for example (Williams, 1985; Clavin and Williams, 1979; Yakhot, 1988; Kerstein et al., 1988; Abdel-Gayed et al., 1988; Aldredge and Williams, 1991; Pocheau, 1994; Aldredge et al., 1998; Kobayashi et al., 2000; Denet, 2001; Veynante and Vervisch, 2002; Lee and Lee, 2003; Bychkov, 2003). Besides, if we forget the complications due to burning, still much controversy remains about turbulence itself even in the simplest classical configurations like flows in tubes (Chen et al., 2003; Hof et al., 2004). For this reason, Shelkin’s explanation of the flame acceleration has not been transformed for a long time into a theory, which could describe the process and predict the acceleration parameters. Moreover, as the combustion science developed further, other candidates for the explanation of accelerating flames appeared such as combustion instabilities, flame acoustics, coupling etc. Another acceleration mechanism was proposed in (Clanet and Searby, 1996), which is coupled to the transition from statistically-spherical to statistically planar geometry of flame propagation on the early stages of burning in tubes just after ignition. This mechanism works also for a very short time; it terminates as soon as the flame touches a tube wall. Finally, in a sequence of papers, Sivashinsky with co-authors has discussed one more mechanism of flame transition to detonation due to the hydraulic resistance, see (Brailovsky et al., 2012) and references therein. The mechanism of hydraulic resistance is one-dimensional, which was already quite different from the intrinsically multi-dimensional scenario proposed by Shelkin.

A noticeable progress in this direction has been achieved during the last decade. First a constructive idea was suggested (Kagan and Sivashinsky, 2003; Ott et al., 2003) that turbulence plays a supplementary role in the acceleration, which is possible even for laminar flames with non-slip at the tube walls. The idea was probed in a few numerical simulation runs and revived the interest to the Shelkin explanation of flame acceleration. It is noted that the idea of laminar flame acceleration is incredibly helpful for the theory because it allows understanding the effect independently of the unsolved problems of turbulent combustion. Unfortunately, the numerical studies (Kagan and Sivashinsky, 2003; Ott et al., 2003) were too limited and provided quite little information beyond the fact that laminar flames can accelerate.

Subsequently, Bychkov et al. (2005) develop the analytical theory of the flame acceleration, which explains the effect and predicts its main tendencies. According to the theory, flames with realistically large density drop at the front
accelerate exponentially from a closed end of a tube with non-slip at the walls. The acceleration is unlimited until a flame triggers a detonation. The analytical formulas for the acceleration rate, for the flame shape and for the velocity profile in the flow pushed by the flame were developed. The theory was validated by extensive numerical simulations. The numerical simulations are performed for the complete set of combustion equations including thermal conduction, viscosity, diffusion and chemical kinetics. The theoretical predictions are in good agreement with the numerical results. However, the theory includes a set of assumptions such as the large Reynolds number related to flame propagation, as well as the large thermal expansion coefficient in the burning process, which in turn leads to the intrinsic limitations of the theory. In this work we determine these limitations and thereby clearly underline the validity domains. Also, the present paper demonstrates the error analysis related to the intrinsic assumptions and accuracy of the theorem.

2. Theory and Methods

Here we briefly recall the theory of (Bychkov et al., 2005). A laminar flame propagating in a 2D tube of half-width \( R \) with adiabatic walls and non-slip at the walls is considered for this theory. In the theory we use the approach of an infinitely thin flame front propagating locally with normal velocity \( U_f \) with respect to the fuel mixture. In 2D geometry, the relative increase in burning rate is simply equal to the rise in the total length of the flame front \( D_f \), such as \( U_w / U_f = D_f / 2R \), where \( U_w \) is the total burning rate and the flame propagation in 2D “volume” of the burning gas rises by \((\Theta-1)2RU_w\) per unit time. Hence, the average velocity is related to the total burning rate as follows

\[
\langle u_z \rangle = (\Theta - 1)U_w.
\]  

Asymptotically, the flame accelerates exponentially in time, \( U_w \propto \exp(\sigma t) \), where the dimensionless acceleration rate \( \sigma \) is an eigenvalue, which has to be obtained from the problem solution. In order to simplify the analytical calculations, we introduce the standard scaling by \( R \), \( U_f \) and \( R/U_f \) as the units of length, velocity and time, respectively. Hence, we arrive to the dimensionless variables \((\eta, \xi) = (x/z)/R\), \( \tau = tU_f/R\), \( w = u/U_f \), \( \Omega_w = U_w/U_f \) and \( \delta_f = D_f/R \). The scaled burning rate is coupled to the scaled length of the flame front as \( \Omega_w = \delta_f / 2 \), the average velocity of the flame-generated flow is \( \langle w_z \rangle = (\Theta - 1)\Omega_w \), and the exponential acceleration of the flame front is described as \( \Omega_w \propto \exp(\sigma \tau) \). A plane-parallel flow ahead of the flame front follows the Navier-Stokes equation

\[
\frac{\partial w_z}{\partial \tau} = -\frac{\partial p}{\partial \xi} + \frac{1}{Re} \frac{\partial^2 w_z}{\partial \eta^2} ,
\]  

where the pressure gradient is generated by the flame front, with the pressure and the density being scaled by \( \rho_f \) and \( \rho_f U_f^2 \), respectively, and \( Re = RU_f / \nu = R / L_f \) Pr is the flame propagation Reynolds number, with the thermal flame thickness \( L_f = D_{th} / U_f \) and the Prandtl number \( \Pr \). Also, considering the exponential state of the flame acceleration, the Navier-Stokes equation for \( w_z(\eta, \tau) = \exp(\sigma \tau)\phi(\eta) \) reduces to an equation for the velocity profile \( \phi(\eta) \)

\[
\mu^2 \phi = C_{II} + \phi^*,
\]  

where
where $\mu = \sqrt{\sigma \text{Re}}$, and the constant $C_{\Pi}$ comes to the equation above due to forcing $\Pi(\tau) = -\partial p / \partial \xi$. Using the non-slip boundary conditions $\varphi = 0$ at $\eta = \pm 1$, we find the solution to Eq. (3)

$$\varphi = \Omega \frac{\cosh \mu - \cosh(\mu \eta)}{\cosh \mu - 1}.$$  (4)

with a more suitable amplitude $\Omega$ introduced instead of the constant $C_{\Pi}$. Then the velocity profile generated by the accelerating flame front is given by

$$w_c = (\Theta - 1) \Omega w \frac{\cosh \mu - \cosh(\mu \eta)}{\cosh \mu - \mu^{-1} \sinh \mu}.$$  (5)

The burning rate is controlled by relative motion of various parts of the flame front. Let us consider that the flat “tip” of the flame at the axis that moves with scaled velocity $1 + w_c(0, \tau)$. We describe the flame shape with respect to the tip-point by the scaled function $f(\eta, \tau) = F / R$ coupled to the scaled flame position $\xi_f(\eta, \tau)$ as $\xi_f = \xi_f(0, \tau) + f(\eta, \tau)$, with $f(0, \tau) = 0$ at the flame tip by the definition. If a segment of the flame front is inclined, then it consumes more fuel mixture per unit time because of the increased surface area as $\sqrt{1 + (\partial f / \partial \eta)^2}$, and thereby it spreads faster. Furthermore, the front segment is drifted by the flow, which leads to its local propagation along the wall with the scaled velocity $w_c + \sqrt{1 + (\partial f / \partial \eta)^2}$, which differs from the flame tip propagation speed. Consequently, the flame shape gets distorted, as a whole, with the following evolution equation

$$-\frac{\partial f}{\partial \tau} = w_c(0, \tau) - w_c + 1 - \sqrt{1 + (\frac{\partial f}{\partial \eta})^2}.$$  (6)

After some transition time we have $(\partial f / \partial \eta)^2 >> 1$ everywhere except for the flat region around the flame tip influencing the burning rate. Assuming symmetry with respect to the axis $\eta = 0$, hereafter we shall consider the domain $\eta > 0$ only, where $\partial f / \partial \eta < 0$ and $\left| \partial f / \partial \eta \right| = -\partial f / \partial \eta$. Equation (6) subsequently acquires the linear type

$$-\frac{\partial f}{\partial \tau} = w_c(0, \tau) - w_c + \frac{\partial f}{\partial \eta}.$$  (7)

We look for the solution to Eq. (7) in the form

$$f(\eta, \tau) = \Phi(\eta) \exp(\sigma \tau).$$  (8)

Then, integrating the flame shape evolution equation, we find

$$\Phi = \frac{(\Theta - 1) \Phi(1)}{\cosh \mu - \mu^{-1} \sinh \mu} \left( \exp(\mu \eta) - \exp(-\mu \eta) \right) + \frac{\mu^2}{2(\mu + \sigma)} \left( \exp(-\sigma \eta) \right) - \frac{1}{\sigma}.$$  (9)

In order to determine the acceleration rate $\sigma$, the condition $\Phi(\eta) = \Phi(1)$ at $\eta = 1$ is used. Then Eq. (9) yields

$$\frac{\mu \cosh \mu - \sinh \mu}{\mu(\Theta - 1)} = \frac{\exp \mu}{2(\mu + \sigma)} - \frac{\exp(-\mu)}{2(\mu - \sigma)} + \frac{\mu^2}{\mu^2 - \sigma^2} \frac{\exp(-\sigma)}{\sigma} - \frac{1}{\sigma}.$$  (10)
Equation (10) couples the flame acceleration rate to the thermal expansion factor $\Theta = \rho_a / \rho_b$ and the flame propagation Reynolds number $Re = RU_f / \nu$. In the limit of large $\Theta$, its leading-order reduction can be solved analytically. Indeed, for $\mu > 1$ Eq. (10) reduces to

$$\mu + \sigma = (\Theta - 1) \frac{\mu}{\mu - 1},$$

with the solution

$$\sigma = \frac{(Re-1)^2}{4Re} \left( 1 + \frac{4Re\Theta}{(Re-1)^2} - 1 \right)^2, \quad \mu = \sqrt{\sigma} Re = \frac{Re-1}{2} \left( 1 + \frac{4Re\Theta}{(Re-1)^2} - 1 \right).$$

In the case of large Reynolds numbers, $Re > 4\Theta$, the result (12) further degenerates to

$$\sigma = \Theta^2 / Re, \quad \mu = \Theta.$$

3. Results and Discussion

While the asymptotical result (12) has been substantiated by direct numerical simulations (Bychkov et al., 2005) for $\mu > 1$, i.e. large $Re$ and $\Theta$, it is quite questionable if one has such good agreement otherwise. Consequently, the main task of the present work is to determine the intrinsic limitations and accuracy of the theory above. For this reason, we have solved Eq. (10) computationally and compare the result obtained to the analytical formula (12) for various $Re$ and $\Theta$. In particular, Fig. 1 compares Eq. (12), solid, Eq. (10), dashed, and direct numerical simulations (DNS) of (Bychkov et al., 2005), markers, to each other, with $\Theta = 8$ in all cases. Here, the simulations for $Pr = 0.5$ and $Pr = 1$ are presented by triangles and circles, respectively. We observe very good agreement between the analytical, Eq. (12), “semi-analytical”, Eq. (10), and DNS predictions in that case.

![FIG. 1. The flame acceleration rate $\sigma$ versus the flame propagation Reynolds number $Re$ at the fixed thermal expansion coefficient $\Theta = 8$. Equations (10) and (12) are shown by dashed and solid lines, respectively, the markers present the direct numerical simulation (Bychkov et al., 2005) for $Pr = 0.5$ (triangles) and $Pr = 1.0$ (circles).](image-url)
However, the results (10) and (12) start deviating from each other as soon as $\Theta$ decreases as clearly shown in Fig. 2, where Eq. (10), dashed, and Eq. (12), solid, are compared for different $\Theta = 4; 6; 8; 10$. The same effect is observed in Fig. 3, where $\sigma$ is plotted versus $\Theta$ for various fixed $Re = 5; 10; 20$. Indeed, while Eq. (12) yields a near-parabolic dependence of $\sigma$ versus $\Theta$ (compare with the asymptotic relation (13)); according to Eq. (10), $\sigma \to 0$ when $\Theta \to 3$. The latter trend also reduces the gap between the present theory and the formulation on steady flame propagation (Akkerman et al., 2010) yielding that a flame surely accelerate in a 2D channel with one end closed if $\Theta > 3$. It is also seen from Fig. 3 that the discrepancy between Eqs. (10) and (12) gets stronger with the decrease in the flame propagation Reynolds number, and thereby one cannot expect a good predictability from the theory in that case.

**FIG. 2.** The flame acceleration rate $\sigma$ versus the flame propagation Reynolds number $Re$ at the fixed thermal expansion coefficients $\Theta = 4; 6; 8; 10$. Equations (10) and (12) are shown by dashed and solid lines, respectively.

**FIG. 3.** The flame acceleration rate $\sigma$ versus the thermal expansion coefficient $\Theta$ at the fixed flame propagation Reynolds numbers $Re = 5; 10; 20$. Equations (10) and (12) are shown by dashed and solid lines, respectively.
We have performed a detailed analysis of such a discrepancy (the “error”) between the computational solution of the comprehensive equation (10) and its analytical approximation (12), as shown in Figs. 4 and 5. Specifically, Fig. 4a shows the error versus $\Theta$ at various fixed $Re = 5; 10; 20$, while the error versus Re at different but fixed $Theta = 4; 6; 8; 10$ is shown in Fig. 4b. It is clearly seen that the error diminishes with the increase in $\Theta$ and/or Re.

FIG. 4a. [Graph showing error versus $\Theta$ at various fixed Re]

FIG. 4b. [Graph showing error versus Re at different fixed $\Theta$]

FIG. 4. Error analysis for $\Theta$ at fixed $Re = 5; 10; 20$ (a) and that for $Re$ at fixed $Theta = 4; 6; 8; 10$ (b).

Eventually, the same result is observed in Fig. 5, where the error isolines (in %) shows the accuracy domains (and thereby the intrinsic limitations of the theory) in the Re-$\Theta$ diagram.

FIG. 5. Contour plot for the overall error analysis.
4. Conclusions

In the present paper the analytical theory of flame acceleration in tubes (Bychkov et al., 2005) is revisited and its intrinsic limitations are determined. While the theory predicts the main feature of flame acceleration rate very well when $\Theta$ and Re are large enough, it may or may not be so accurate at other conditions. We can say for sure that these assumptions may not be acceptable everywhere, and the intrinsic limitations and the accuracy are eventually determined in the Re-$\Theta$ diagram in Fig. 5. It is demonstrated that the accuracy is improved while $\Theta$ and Re increases.

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