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Transition from pulled to pushed fronts in premixed turbulent combustion: Theoretical and numerical study

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ABSTRACT

This paper extends a previous theoretical study (Sabelnikov and Lipatnikov, 2013) of the influence of countergradient transport (CGT) on the speed of a statistically stationary, planar, 1D premixed flame that passively propagates in homogenous turbulence in the form of a traveling wave, i.e. retains its mean thickness and structure. While two particular models of the mean rate of product creation were addressed in the previous article, with the shape of the rate as a function of the Favre-averaged combustion progress variable being concave in both cases, the present paper deals with a more general model that subsumes both concave functions and functions with an inflection point, i.e. a point where the function changes from being concave to convex or vice versa. In this more general case, transition from pulled (flame speed is controlled by processes localized to the flame leading edge) to pushed (flame speed is controlled by processes within the entire flame brush) flames can occur both due to interplay of the nonlinear reaction term and a nonlinear convection term associated with CGT and due to the change of the shape of the reaction term in the absence of CGT. Explicit pushed traveling wave solutions to the studied problem are theoretically derived and conditions under that developing flames approach either pushed or pulled traveling wave solution are obtained by analyzing the governing equations at the flame leading edge and invoking the steepness selection criterion which highlights traveling wave with the steepest profile at the leading edge. Other analytical results include conditions for transition from pulled to pushed premixed turbulent flames, dependence of flame speed on the magnitude of the CGT term and the shape of the mean reaction rate, analytical expressions for the mean thickness of the pushed flames and turbulent scalar flux within the pushed flames. All these theoretical findings are validated by results of unsteady numerical simulations of the initial boundary value problem with steep initial wave profiles.

1. Introduction

Due to extreme complexity of various highly nonlinear and multiscale phenomena associated with premixed turbulent combustion, its theoretical analysis is commonly simplified to a study of propagation of a statistically stationary, planar, 1D premixed flame in homogeneous turbulence which is not affected by the flame. Moreover, in such theoretical studies, the state of the mixture is often characterized with a single scalar variable c called combustion progress variable ($c = 0$ and $c = 1$ in unburned mixture and combustion products, respectively) and the flame propagation is modeled with a single balance equation [1]

$$\bar{\rho}\frac{\partial \tilde{c}}{\partial t} + \bar{\rho}\tilde{u}\frac{\partial \tilde{c}}{\partial x} + \frac{\partial \overline{\rho u'' c''}}{\partial x} = \overline{W}(\tilde{c}), \tag{1}$$

which involves two unclosed terms; turbulent scalar flux $F_t = \overline{\rho u'' c''}$ and the mean mass rate $\overline{W}$ of product creation. Here, t is the time, x and u are a spatial coordinate and the flow velocity, respectively, ρ is the gas density, $\tilde{q} = \overline{\rho q}/\bar{\rho}$ and $q'' = q - \tilde{q}$ designate the Favre-averaged and fluctuating quantities, respectively, with the Reynolds averages being denoted with over-bars, e.g. $\bar{\rho}$.

If the turbulent scalar flux in Eq. (1) is closed by invoking the gradient transport (GT) approximation

$$F_t = \overline{\rho u'' c''} = -\bar{\rho} D_t \frac{\partial \tilde{c}}{\partial x}, \tag{2}$$

where $D_t > 0$ is a turbulent diffusion coefficient, then, Eq. (1) belongs to a wide class of partial differential equations, which are called convection–diffusion–reaction (CDR) equations. Such

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equations are widely studied in various fields of science starting from the pioneering work by Fisher [2] and Kolmogorov et al. [3] who developed the well-known KPP theory of such equations.

More precisely, Kolmogorov et al. [3] considered a diffusion–reaction (DR) equation, which results from Eqs. (1) and (2) in the case of $\tilde{u}=0$, a constant D_t, and a constant density. They also assumed a concave, i.e. $W[(\tilde{c}_1+\tilde{c}_2)/2] > [W(\tilde{c}_1)+W(\tilde{c}_2)]/2$ for any $0 \leqslant \tilde{c}_1 < \tilde{c}_2 \leqslant 1$, "hump"-like shape of the source term in the DR equation, i.e. $\overline{W}(\tilde{c})$ in Eq. (1), with the highest slope $d\overline{W}/d\tilde{c}$ being reached at $\tilde{c}=0$. Moreover, $\overline{W}(0)=\overline{W}(1)=0$ and $\overline{W}(\tilde{c})>0$ if $0<\tilde{c}<1$. Logistic expression $\tilde{c}(1-\tilde{c})$ and term $\tilde{c}-\tilde{c}^q$ with $q>1$ are well-known simple examples of such a concave source term multiplied with a proper time scale. Kolmogorov et al. [3] sought for permanent monotonous traveling wave (TW) solutions $\tilde{c}(x,t)=\tilde{c}(X)$, where $X=x+u_0t$, to the studied DR equation with the boundary conditions of $\tilde{c}(-\infty)=0$ and $\tilde{c}(+\infty)=1$. Such a TW solution satisfies the following ordinary differential equation (ODE)

$$u_0\frac{d\tilde{c}}{dX}=D_t\frac{d^2\tilde{c}}{dX^2}+\overline{W}(\tilde{c}), \tag{3}$$

retains its shape $\tilde{c}(X)$, and moves at a constant speed u_0. Kolmogorov et al. [3] have analytically solved this nonlinear boundary value problem (BVP) and have proved that it does not have a unique solution, i.e. there is a family of TW solutions and a continuous spectrum of eigenvalues, i.e. the TW speeds u_0, bounded with a minimum (slowest) speed $u_{0,KPP}=\sqrt{2D_t\overline{W}'(0)}$ where $\overline{W}'(\tilde{c})=d\overline{W}/d\tilde{c}$. The constraint of $u_0 \geqslant u_{0,KPP}$ has been obtained by linearizing the ODE at the leading edge $\tilde{c}\to 0$ (an unstable state) of a TW. Moreover, Kolmogorov et al. [3] analytically studied the initial boundary value problem (IBVP) with localized initial conditions, i.e. $\tilde{c}(x,t=0)=\tilde{c}_0(x)$, with $\tilde{c}_0(x)$ being a monotonously increasing function in an interval of $x_1<x<x_2$, but $\tilde{c}_0(x)=0$ if $x<x_1$ and $\tilde{c}_0(x)=1$ if $x>x_2>x_1$. A step function $H(x-x_1)$ is a particular case of such an initial profile $\tilde{c}_0(x)$ with $x_1=x_2$. Finally, Kolmogorov et al. [3] have solved the speed selection problem and have proved that solutions to the IBVP approach the TW solution characterized by the slowest propagation speed provided that the initial wave profiles are steep enough, e.g. the step function. TW solutions found by Kolmogorov et al. [3] are called "pulled" waves [4,5] in order to stress that the speed of such a solution is determined from the linear analysis of the problem at the unstable state $\tilde{c}\ll 1$, i.e. the TW is pulled by its leading edge.

In the combustion literature, the KPP approach was widely applied to the CDR equation that results from Eqs. (1) and (2) in order to determine fully developed turbulent burning velocity U_t [6–14], which was associated with the slowest TW speed in the cited papers. Various expressions for U_t were obtained in Refs. [6–14] depending on invoked closure relation for the mean rate $\overline{W}(\tilde{c})$, but U_t was controlled by D_t and the slope of $\overline{W}(\tilde{c})$ at $\tilde{c}\to 0$ in all these studies.

It is worth noting, however, that the source term in the DR equation is not necessary to be a concave function in a general case. The maximum slope of $\overline{W}(\tilde{c})$ can be reached inside the interval of $0<\tilde{c}<1$ and the source term can have an inflection point, where the dependence of $\overline{W}$ on $\tilde{c}$ changes from being concave to convex, i.e. $W[(\tilde{c}_1+\tilde{c}_2)/2] < [W(\tilde{c}_1)+W(\tilde{c}_2)]/2$ for any $0 \leqslant \tilde{c}_1 < \tilde{c}_2 \leqslant 1$, or vice versa. Such a case was studied by Aronson and Weinberger [15] who have proved that the BVP for Eq. (3) has a solution for any $u_0 \geqslant u_{0,\min} \geqslant u_{0,KPP}=\sqrt{2D_t\overline{W}'(0)}$, but, contrary to the KPP case, the slowest speed $u_{0,\min}$ cannot be found by linearizing Eq. (3) at $\tilde{c}\ll 1$. They have proved also that TW solutions characterized by a continuous spectrum of $u_0>u_{0,\min}$ are pulled, whereas, if $u_{0,\min}>u_{0,KPP}$, then, the TW solution with $u_0=u_{0,\min}$ is basically different, i.e. it has the steepest profile of $\tilde{c}(X)$ at $\tilde{c}\to 0$, with the speed $u_{0,\min}$ being controlled by processes in the entire wave. Such a TW solution is called pushed wave [4,5]. Examples of pushed waves that are modeled by CDR equations with ρ = const, $\tilde{u}=0$, and source terms that are convex somewhere within the interval of $0<\tilde{c}<1$ can be found e.g. in Refs. [16–18]. Aronson and Weinberger [15] have also solved the speed selection problem and have shown that a solution to the IBVP associated with Eqs. (1) and (2) approaches the TW solution characterized by the slowest propagation speed $u_{0,\min}$ provided that the initial wave profile is steep enough, e.g. the step function. If applied to premixed turbulent combustion, the general mathematical result by Aronson and Weinberger [15] indicates that the KPP approach cannot be used to determine U_t if an invoked closure relation for $\overline{W}(\tilde{c})$ has an inflection point in the interval of $0<\tilde{c}<1$.

A laminar premixed flame modeled with the following CDR equation

$$\rho\frac{\partial c}{\partial t}+\rho u\frac{\partial c}{\partial x}=\frac{\partial}{\partial x}\left(\rho D\frac{\partial c}{\partial x}\right)+\frac{\rho\Phi(c)}{\tau_0}\times\exp\left[-\frac{Ze(1-c)}{1-(1-\sigma^{-1})(1-c)}\right], \tag{4}$$

where $\Phi(c)=0$ at $0\leqslant c\leqslant c_1<1$ and $Ze\gg 1$, is another well-known example of a pushed TW, as shown by Zeldovich and Frank-Kamenetsky [19–21]. Here, $c=(T-T_u)/(T_b-T_u)$ is the normalized temperature, $Ze=(T_b-T_u)E/(R_0T_b^2)$ is the Zeldovich number, T_u and T_b designate temperatures of unburned and burned gases, respectively, E is the activation temperature of a single global reaction that combustion chemistry is reduced to, R_0 is the universal gas constant, D is molecular diffusivity, τ_0 is a reaction time scale, $\Phi(c)$ is a weakly non-linear (when compared to the Arrhenius exponential term) function such that $\Phi(c_1<c<1)>0$ and $\Phi(1)=0$, and $\sigma=T_b/T_u$. The KPP theory is not applicable to this problem, because $d\Phi/dc=0$ at the leading edge, and there is a single TW solution [19–21]. In the case of $\Phi(0\leqslant c<1)>0$, Eq. (4) can have an intermediate asymptotic solution [21–23], which retains its shape and speed over a long time interval and is associated with a pushed or pulled wave if $\sigma-1$ is much larger than or on the order of R_0T_b/E, respectively, with the speed of the pulled flame being consistent with the KPP theory.

As far as premixed turbulent combustion is concerned, transition from pulled to pushed TWs is straightforwardly relevant to the following long-standing basic issue. On the one hand, production of flamelet surface area within a premixed turbulent flame brush is often considered to control its speed including the speed of its leading edge [24,25]. On the other hand, within the framework of the leading point concept pioneered by Zeldovich [26], see also pp. 450–452 in Ref. [21], the mean turbulent flame speed is hypothesized to be controlled by processes localized to the leading edge of the mean flame brush, whereas the production of flamelet surface area within the flame brush adjusts itself to the speed of the leading edge. The readers interested in further discussion of the leading point concept and facts that indirectly support it are referred to books [27,28], a review paper [29], and recent contributions by Lieuwen et al. [30–34].

To the best of the present authors knowledge, TW solutions to Eqs. (1) and (2) have not yet been investigated analytically in the case of $\overline{W}(\tilde{c})$ with an inflection point at $0<\tilde{c}<1$ in the turbulent combustion literature. The major goal of the present work is to fill this gap. Moreover, the following issue specific to turbulent flames will also be addressed.

As predicted by Clavin and Williams [35] and Bray and Libby [36], experimentally discovered by Moss [37] and by Yanagi and Mimura [38], and documented in a number of subsequent experimental and direct numerical simulation (DNS) studies reviewed