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LETTER TO THE EDITOR

Reaction front propagation in a turbulent flow

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Abstract. The large-scale dynamics of a reaction front in a turbulent flow in the limit of large Reynolds number has been studied starting from the Kolmogorov–Petrovskii–Piskunov equation, modified by the random convection term. Random velocity has been assumed to be a homogeneous Gaussian field with Kolmogorov energy spectrum and infrared divergence. An upper bound for the position and speed of the reaction front in the long-time, large-distance limit has been derived by the method of random characteristics and a renormalization procedure. It has been shown that the infrared divergence of the random velocity field leads to the acceleration of a coarse-grained reaction front.

Reaction front propagation in a turbulent flow is a problem of considerable significance both for applications in combustion science and also for understanding the nature of turbulence itself. It has been investigated by many authors using different techniques and methods (for a recent review see [1]). The main purpose of such studies is the determination of the turbulent burning velocity, which is the overall propagation rate at which a reaction front propagates throughout a turbulent flow. The big progress in this area has been achieved by applying the so-called G-equation, describing the front propagation by the Huygens mechanism [2–10]. This equation, has been studied using numerical methods [4, 5], renormalization-group approach [6, 7], scaling analysis [8, 9], and the path-integral approach [10] proved to be very useful in the determination of the turbulent burning velocity.

In this paper we present an alternative approach to the problem of reaction front propagation in a random velocity field which is also based on a geometric optics approximation but is different in many important aspects. We develop an equation describing the long-time, large-distance behaviour of a reaction front, *starting* with a nonlinear equation of Kolmogorov–Petrovsii–Piskunov (KPP) type with a random convection term. Our primary interest is to describe the front propagation on length and time-scales that are larger than the integral length scale of turbulence, l_0, and the turnover time-scale $t_0 \sim l_0/u_0$, where u_0 is the typical velocity of the energy containing eddies of the turbulence. The procedure used is an adaptation of the functional integral technique, which has been used by Freidlin and Gärtner for studying nonlinear reaction–diffusion equations [11–14], and of exact renormalization theory for turbulent transport, which has been developed by Avellaneda and Majda [15, 16].

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Let us start with a non-dimensional equation for a scalar field $\varphi(t, x)$

$$\frac{\partial\varphi}{\partial t} + v(t, x) \cdot \nabla\varphi = D\nabla^2\varphi + c(\varphi)\varphi \qquad x \in \mathbf{R}^3 \tag{1}$$

where the velocity $v(t, x)$ is assumed to be a homogeneous random field with zero mean and the nonlinear source term $c(\varphi)\varphi$ is of KPP type, i.e.

$$c \equiv c(0) = \max_{\varphi\in[0,1]} c(\varphi) > 0 \qquad c(1) = 0\,. \tag{2}$$

Here the Kolmogorov length scale $\eta = (\nu^3/\bar{\varepsilon})^{1/4}$, velocity scale $v_k = (\nu\bar{\varepsilon})^{1/4}$ and time-scale $t_k = \nu/v_k$ are used as units of space coordinates, velocity and time, respectively; $\bar{\varepsilon}$ is the average dissipation rate. The diffusion coefficient is non-dimensionalized by the viscosity ν.

The initial condition is

$$\varphi(0, x) = g(x) = \begin{cases} 1 & \text{if} \quad x \in \Omega \\ 0 & \text{otherwise}\,. \end{cases} \tag{3}$$

It should be noted that (1) has been studied by Souganidis and Majda [17] for a random velocity field involving two separated length scales. Here we will be concerned with a random flow with arbitrary many spatial scales.

It can be expected that the macroscale front dynamics for (1)–(3) will be described through an effective equation with the effective parameters depending on the statistical characteristics of the random velocity field $v(t, x)$. We propose the following formula determining the reaction front position in the long-time large-distance limit:

$$S_G = \{x \in \mathbf{R}^3 : G(t, x) = 0\}$$

where

$$G(t, x) = \lim_{\epsilon\to 0} \lambda(\epsilon) \ln\left\langle \varphi^*\left(\frac{t}{\lambda(\epsilon)}, \frac{x}{\epsilon}\right)\right\rangle \tag{4}$$

and φ^* is a solution of (1)–(3) when $c(\varphi)$ is replaced by its maximum value c. Here the angular brackets $\langle\cdot\rangle$ denote the ensemble averaging over velocity statistics and $\lambda(\epsilon)$ is a positive function such that $\lim_{\epsilon\to 0} \lambda(\epsilon) = 0$. The small parameter ϵ is taken to be the ratio of the Kolmogorov length scale η to the integral length scale l_0, that is $\epsilon = Re^{-3/4}$, where $Re = u_0 l_0/\nu$ is a Reynolds number. The scaling function $\lambda(\epsilon)$ has to be determined under the condition of existence of a non-trivial limit (4) and this problem is analogous to that of determining nonlinear rescaling in the exact renormalization theory for turbulent transport [15, 16]. The manifold S_G can be interpreted as a reaction front when

$$\lim_{\epsilon\to 0}\left\langle \varphi\left(\frac{t}{\lambda(\epsilon)}, \frac{x}{\epsilon}\right)\right\rangle = \begin{cases} 1 & G(t, x) > 0 \\ 0 & G(t, x) < 0\,. \end{cases}$$

To illustrate the basic ideas presented in this paper, it is instructive to first consider a special case of the problem (1)–(3), namely the one-dimensional KPP equation

$$\frac{\partial \varphi}{\partial t} = D\frac{\partial^2 \varphi}{\partial x^2} + c(\varphi)\varphi \qquad -\infty < x < \infty \tag{5}$$

with the initial condition

$$\varphi(0,x) = \chi(x) = \begin{cases} 1 & x \leqslant 0 \\ 0 & x > 0 . \end{cases} \tag{6}$$

It is well known that the function $\varphi^\epsilon(t,x) = \varphi(t/\epsilon, x/\epsilon)$ tends, as $\epsilon \to 0$, to a progressive wave $\chi(x - ut)$ travelling on the positive x-direction with constant speed $u = (4cD)^{1/2}$. Freidlin was the first to treated the problem (5), (6) and its generalizations by means of functional integrals [11–14]. Let us reformulate the Freidlin treatment of the KPP equation by using an alternative approach which is particularly suited for our further consideration. Instead of equations (5) and (6), let us consider an auxiliary first-order differential equation

$$\frac{\partial \varphi_v}{\partial t} = v(t)\frac{\partial \varphi_v}{\partial x} + c(\varphi_v)\varphi_v \qquad -\infty < x < \infty \tag{7}$$

with the initial condition

$$\varphi_v(0,x) = \chi(x) \tag{8}$$

where the auxiliary random process $v(t)$ is a white Gaussian noise with a probability density functional of the form

$$P[v] = \exp\left(-\frac{1}{4D}\int v^2(s)\,\mathrm{d}s\right). \tag{9}$$

Let us show now that in the limit $\epsilon \to 0$, the ensemble average

$$\langle \varphi_v^\epsilon(t,x)\rangle = \left\langle \varphi_v\left(\frac{t}{\epsilon}, \frac{x}{\epsilon}\right)\right\rangle$$

tends to the unit step function $\chi(x - ut)$ and the function

$$G(t,x) = \lim_{\epsilon\to 0} \epsilon \ln\left\langle \varphi_v^*\left(\frac{t}{\epsilon}, \frac{x}{\epsilon}\right)\right\rangle \tag{10}$$

determines the position of the wavefront (compare with (4)). Applying the scaling transformation $t \to t/\epsilon, x \to x/\epsilon$ to (7) and (8), we can get

$$\frac{\partial \varphi_v^\epsilon}{\partial t} = v\left(\frac{t}{\epsilon}\right)\frac{\partial \varphi_v^\epsilon}{\partial x} + \frac{c(\varphi_v^\epsilon)}{\epsilon}\varphi_v^\epsilon \qquad \varphi_v^\epsilon(0,x) = \chi(x). \tag{11}$$

It follows from the method of characteristics that the solution of (11) is given by the integral equation

$$\varphi_v^\epsilon(t,x) = \chi\left(x + \int_0^t v\left(\frac{s}{\epsilon}\right)\mathrm{d}s\right)\exp\left[\frac{1}{\epsilon}\int_0^t c\left(\varphi_v^\epsilon(s, x + \int_s^t v\left(\frac{\tau}{\epsilon}\right)\mathrm{d}\tau\right)\mathrm{d}s\right]. \tag{12}$$

Using equations (9), (12) and $c(\varphi) \leqslant c$, we find that

$$\langle \varphi_v^\epsilon(t,x)\rangle = \int \varphi_v^\epsilon(t,x)P[v]\mathcal{D}v(t) \leqslant \left\langle \varphi^*\left(\frac{t}{\lambda(\epsilon)},\frac{x}{\epsilon}\right)\right\rangle$$
$$= \exp\left(\frac{ct}{\epsilon}\right)\int \chi\left(x+\int_0^t v\left(\frac{\tau}{\epsilon}\right)\mathrm{d}\tau\right)P[v]\mathcal{D}v(t)$$
$$= \frac{1}{(4\pi D\epsilon t)^{1/2}}\int_{-\infty}^0 \exp\left(\frac{ct}{\epsilon}-\frac{(x-\xi)^2}{4D\epsilon t}\right)\mathrm{d}\xi \propto \exp\left(\frac{G(t,x)}{\epsilon}\right) \tag{13}$$

where

$$G(t,x) = ct - \frac{x^2}{4Dt}.$$

One may conclude from this bound that $\lim_{\epsilon\to 0}\langle\varphi_v^\epsilon(t,x)\rangle = 0$ provided that $G(t,x) < 0$. One can also find that $\lim_{\epsilon\to 0}\langle\varphi_v^\epsilon(t,x)\rangle = 1$ when $G(t,x) > 0$ [14]. This means that an equation $G(t,x) = 0$ gives us a position of front $x(t) = (4cD)^{1/2}t$ and its propagation rate $\dot{x}(t) = (4cD)^{1/2}$.

The question arises as to whether this simple analysis can be adapted and extended to the random-advection problem (1)–(3), with a view of determining the coarse-grained position and speed of a reaction front as $\epsilon \to 0$. This is a very difficult problem and therefore it is reasonable to consider this problem under the simplest but non-trivial conditions. In this paper we assume that the velocity $\boldsymbol{v}$ is a Gaussian random field of the form [15, 16]

$$\boldsymbol{v} = (0, v(t,x), 0) \tag{14}$$

with a zero mean and a correlation function with Kolmogorov spectrum given by

$$\langle v(t,x)v(t',x')\rangle = \frac{1}{\sqrt{2\pi}}\int \exp\{\mathrm{i}k(x-x') - a|k|^{2/3}|t-t'|\}\psi_0\left(\frac{|k|}{\epsilon}\right)\psi_\infty(|k|)|k|^{-5/3}\,\mathrm{d}k \tag{15}$$

where $\psi_0(z)$ and $\psi_\infty(z)$ represent infrared and ultraviolet cut-offs and satisfy

$$\psi_0(z) = \begin{cases} 0 & \text{if } |z| < z_0 \\ 1 & \text{if } |z| > z_1 \end{cases} \qquad \psi_\infty(z) = \begin{cases} 1 & \text{if } |z| < z_3 \\ 0 & \text{if } |z| > z_4. \end{cases} \tag{16}$$

An important feature of this random velocity field is the infrared divergence of energy since $\langle v^2\rangle \to \infty$ as $\epsilon \to 0$.

Although the model (14)–(16) is not a particularly realistic description of a turbulent flow, we think that its simplicity enables us to determine many of the important features of reaction front propagation in a random velocity field analytically, but, perhaps more importantly, it helps us to identify the basic physics mechanisms that lead to the acceleration of a flame front (see equation (31)).

The problem defined by (1)–(3) and (14)–(16) requires the solution of the nonlinear stochastic PDE. However, one may conclude from (13) that the limit $\epsilon \to 0$ allows us to determine the upper bound for the position and propagation rate of a reaction front for the nonlinear problem (5) and (6) considering only linear approximation. For this reason, in what follows, we consider instead of (1)–(3) a linear equation

$$\frac{\partial \varphi}{\partial t} + v(t,x)\frac{\partial \varphi}{\partial y} = v_x(t)\frac{\partial \varphi}{\partial x} + v_y(t)\frac{\partial \varphi}{\partial y} + c\varphi \tag{17}$$

with initial condition

$$\varphi(0,x,y) = \chi(y) = \begin{cases} 1 & y \leqslant 0 \\ 0 & y > 0\,. \end{cases} \tag{18}$$

The independent zero-mean white Gaussian noises $v_x(t)$ and $v_y(t)$ are chosen to have the same value of noise intensity parameter as a diffusion coefficient D in (1):

$$\langle v_x(t)v_x(t')\rangle = 2D\delta(t-t') \qquad \langle v_y(t)v_y(t')\rangle = 2D\delta(t-t')\,. \tag{19}$$

We wish now to find the upper bound for the macroscale position and speed of a reaction front propagating in the positive y-direction. Consider a scaling transformation

$$t \to \frac{t}{\lambda(\epsilon)} \qquad x \to \frac{x}{\epsilon} \qquad y \to \frac{y}{\epsilon}\,.$$

After rescaling one can get an equation for

$$\varphi^{\epsilon}(t,x,y) = \varphi\left(\frac{t}{\lambda},\frac{x}{\epsilon},\frac{y}{\epsilon}\right)$$

in the following form:

$$\frac{\partial \varphi^{\epsilon}}{\partial t} + \frac{\epsilon}{\lambda}v\left(\frac{t}{\lambda},\frac{x}{\epsilon}\right)\frac{\partial \varphi^{\epsilon}}{\partial y} = \frac{\epsilon}{\lambda}v_x\left(\frac{t}{\lambda}\right)\frac{\partial \varphi^{\epsilon}}{\partial x} + \frac{\epsilon}{\lambda}v_y\left(\frac{t}{\lambda}\right)\frac{\partial \varphi^{\epsilon}}{\partial y} + \frac{c}{\lambda}\varphi^{\epsilon}\,. \tag{20}$$

Let $\varphi^{\epsilon}_{\xi}(t,x)$ be the Fourier transformation of $\varphi^{\epsilon}(t,x,y)$ in the variable y

$$\varphi^{\epsilon}(t,x,y) = \frac{1}{\sqrt{2\pi}}\int \varphi^{\epsilon}_{\xi}(t,x)\mathrm{e}^{\mathrm{i}y\xi}\,\mathrm{d}y\,. \tag{21}$$

Then the transformation of (20) yields

$$\frac{\partial \varphi^{\epsilon}_{\xi}}{\partial t} + \mathrm{i}\xi\frac{\epsilon}{\lambda}v\left(\frac{t}{\lambda},\frac{x}{\epsilon}\right)\varphi^{\epsilon}_{\xi} = \frac{\epsilon}{\lambda}v_x\left(\frac{t}{\lambda}\right)\frac{\partial \varphi^{\epsilon}_{\xi}}{\partial x} + \mathrm{i}\xi\frac{\epsilon}{\lambda}v_y\left(\frac{t}{\lambda}\right)\varphi^{\epsilon}_{\xi} + \frac{c}{\lambda}\varphi^{\epsilon}_{\xi}\,. \tag{22}$$

This equation can easily be solved by the method of characteristics. The stochastic characteristic curves are

$$x(t) = x - \frac{\epsilon}{\lambda}\int_0^t v_x\left(\frac{s}{\lambda}\right)\mathrm{d}s$$

and the solution φ^{ϵ}_{ξ} is given by

$$\varphi^{\epsilon}_{\xi}(t,x) = \varphi^{\epsilon}_{\xi}(0)\exp\left\{\frac{ct}{\lambda} - \mathrm{i}\xi\frac{\epsilon}{\lambda}\int_0^t\left(v\left(\frac{s}{\lambda},\frac{x}{\epsilon}+\frac{1}{\lambda}\int_s^t v_x\left(\frac{\tau}{\lambda}\right)\mathrm{d}\tau\right) + v_y\left(\frac{s}{\lambda}\right)\right)\mathrm{d}s\right\}. \tag{23}$$

Applying the Fourier inverse transformation, we have

$$\varphi^\epsilon(t,x,y) = \frac{1}{2\pi}\int\int e^{i(z-y)\xi}\chi(z)\exp\left\{\frac{ct}{\lambda} - i\xi\frac{\epsilon}{\lambda}\int_0^t\left(v\left(\frac{s}{\lambda},\frac{x}{\epsilon}+\frac{1}{\lambda}\int_s^t v_x\left(\frac{\tau}{\lambda}\right)d\tau\right)\right.\right.$$
$$\left.\left. + v_y\left(\frac{s}{\lambda}\right)\right)ds\right\}d\xi\,dz. \tag{24}$$

Now let us find an average value $\langle\varphi^\epsilon(t,x,y)\rangle$. Since $v(t,x)$, $v_x(t)$ and $v_y(t)$ are assumed to be statistically independent, the average $\langle\cdot\rangle$ can be thought of as three independent averages over $v(t,x)$, v_x and v_y. By using the well known formula for zero-mean Gaussian variables $\langle\exp\xi\rangle = \exp(\langle\xi^2\rangle/2)$ we obtain

$$\langle\varphi^\epsilon(t,x,y)\rangle = \frac{1}{2\pi}\int\int e^{i(z-y)\xi}\chi(z)\left\langle\exp\left\{\frac{ct}{\lambda} - \xi^2\lambda S_\epsilon(t)\right\}\right\rangle d\xi\,dz \tag{25}$$

where

$$S_\epsilon(t) = \frac{\epsilon^2}{2\lambda^3}\left[\int_0^t\int_0^t\left(\left\langle v\left(\frac{s}{\lambda},\frac{x}{\epsilon}+\frac{1}{\lambda}\int_s^t v_x\left(\frac{\tau}{\lambda}\right)d\tau\right)v\left(\frac{s'}{\lambda},\frac{x}{\epsilon}+\frac{1}{\lambda}\int_{s'}^t v_x\left(\frac{\tau}{\lambda}\right)d\tau\right)\right\rangle\right.\right.$$
$$\left.\left. + \frac{1}{\lambda}\left\langle v_y\left(\frac{s}{\lambda}\right)v_y\left(\frac{s'}{\lambda}\right)\right\rangle\right)ds\,ds'\right]. \tag{26}$$

If we introduce into this formula the relations (15) and (19) we obtain

$$S_\epsilon(t) = \frac{\epsilon^2}{2\sqrt{2\pi}\lambda^3}\int_0^t\int_0^t\int\exp\left\{\frac{ik}{\lambda}\int_s^{s'} v_x\left(\frac{\tau}{\lambda}\right)d\tau - \frac{a|k|^{2/3}}{\lambda}|s-s'|\right\}$$
$$\psi_0\left(\frac{|k|}{\epsilon}\right)\psi_\infty(|k|)|k|^{-5/3}\,dk\,ds\,ds' + \frac{\epsilon^2 Dt}{\lambda^2}. \tag{27}$$

This equation implies that $\langle\varphi^\epsilon\rangle$ is independent of x.

Now we are in a position to find the limit of $\langle\varphi^\epsilon\rangle$ as $\epsilon\to 0$ and thereby the equation determining the upper bound for the position and speed of a macroscale reaction front. First, the infrared divergent integral in (27) which occurs in the limit $\epsilon\to 0$ has to be rendered finite. In this case, a renormalization procedure can be set up, analogous to that described in [15, 16] and with the same conclusion, that infrared divergence of the velocity field (14)–(16) leads to a new scaling law $\lambda(\epsilon)$.

Since the integral

$$\int\psi_0(|k|)|k|^{-5/3}\,dk$$

is convergent, the wavenumber k should be rescaled as $k\to\epsilon k$.

Then

$$S_\epsilon(t) = \frac{\epsilon^{4/3}}{2\sqrt{2\pi}\lambda^3}\int_0^t\int_0^t\int\exp\left\{\frac{i\epsilon k}{\lambda}\int_s^{s'} v_x\left(\frac{\tau}{\lambda}\right)d\tau - \frac{a\epsilon^{2/3}|k|^{2/3}}{\lambda}|s-s'|\right\}$$
$$\times\,\psi_0(|k|)\psi_\infty(\epsilon|k|)|k|^{-5/3}\,dk\,ds\,ds' + \frac{\epsilon^2 Dt}{\lambda^2}.$$

It is now apparent that the function $S_\epsilon(t)$ has a non-trivial limit as $\epsilon \to 0$, when

$$\lambda(\epsilon) = \epsilon^{4/9} \tag{28}$$

so that

$$S_0(t) = \lim_{\epsilon\to 0} S_\epsilon(t) = D_v t^2 \tag{29}$$

where

$$D_v = \frac{1}{2\sqrt{2\pi}} \int \psi_0(|k|)|k|^{-5/3}\, \mathrm{d}k\,.$$

Since $\lim_{\epsilon\to 0} \epsilon/\lambda(\epsilon) = 0$, the contribution from the white Gaussian noises $v_x(t)$ and $v_y(t)$ is negligible. This result agrees, of course, with that obtained in [15] by using the Feynman–Kac formula.

Using equations (25) and (29) we find

$$G(t, y) = \lim_{\epsilon\to 0} \lambda(\epsilon) \ln\left\langle \varphi\left(\frac{t}{\lambda(\epsilon)}, \frac{y}{\epsilon}\right)\right\rangle = ct - \frac{y^2}{4S_0(t)}\,. \tag{30}$$

This can be regarded as the equation which determines the upper bound for the position $y(t)$ and the propagation rate $u(t)$ of a reaction front in the long-time large-distance limit. By equating $G(t, y)$ to zero, we find

$$y(t) = (4cD_v t^3)^{1/2} \qquad u(t) = \frac{\mathrm{d}y}{\mathrm{d}t} = 3(cD_v t)^{1/2}\,. \tag{31}$$

Clearly, in the limit $\epsilon \to 0$, the 'reaction zone' shrinks to the surface dividing the space into two regions, so that

$$\lim_{\epsilon\to 0}\left\langle \varphi\left(\frac{t}{\lambda(\epsilon)}, \frac{y}{\epsilon}\right)\right\rangle = \begin{cases} 1 & y < y(t) \\ 0 & y > y(t)\,. \end{cases} \tag{32}$$

It should be noted that the relation

$$\lim_{\epsilon\to 0}\left\langle \varphi\left(\frac{t}{\lambda(\epsilon)}, \frac{y}{\epsilon}\right)\right\rangle = 1$$

remains to be proved rigorously.

The question is what relevance do the results obtained here have to experimental studies of front propagation? In the combustion literature, for example, one can find a discussion on the existence of a stationary turbulent burning velocity, since there is some experimental evidence of the continual growth of turbulent burning rate with time [1]. The results can also be considered as a quantitative description of the mechanism by which the random velocity field accelerates the reaction front and thereby creates the conditions for the occurence of something like the deflagration-to-detonation transition [18].

To summarize, we have derived the upper bound for the position and propagating rate of a large-scale reaction front by using the method of random characteristics and renormalization procedure. Our basic model was defined to include the KPP equation modified by the simple shearing motion with a stationary Gaussian random field exhibiting an infrared divergence in the high Reynolds number limit. The main physical result is that the infrared divergence of velocity field (14)–(16) leads to the acceleration of a macroscale reaction front ($u(t) \sim t^{1/2}$). Clearly, this phenomenon is physically due to the increase of the transport process by enhanced time-dependent diffusion $D_v t$ in the y-direction, which dominates the molecular diffusion and yields faster front propagation.

To conclude, we wish to point out that the analysis presented here can be extended to the more complex statistics of velocity field [15, 16]. It would be very interesting to take into account the possible crossover between different scaling regimes as the spectral parameters of a random velocity field are varied. This is clearly of major interest for our understanding of the large-scale dynamics of reaction fronts in a fully developed turbulent flow.

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